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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L1 15163 SEA FILE=REGISTRY ABB=ON PLU=ON GGGF/SQSP  
L4 56 SEA FILE=REGISTRY ABB=ON PLU=ON L1 AND SQL=4  
L5 42 SEA FILE=HCAPLUS ABB=ON PLU=ON L4

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=> d ibib abs hitrn 15 1-42

L5 ANSWER 1 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:434299 HCAPLUS

DOCUMENT NUMBER: 139:30773

TITLE: Peptides that bind to p185, and methods for the treatment and diagnosis of tumors

INVENTOR(S): Greene, Mark I.; Murali, Ramachandran; Berezov, Alan

PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.    | KIND   | DATE     | APPLICATION NO. | DATE     |
|---------------|--|----------|-----------------|----------|
| WO 2003045309 | A2   | 20030605 | WO 2002-US37390 | 20021121 |
| W:            | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |          |                 |          |
| RW:           | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,  |          |                 |          |

CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,  
NE, SN, TD, TG

US 2003148932 A1 20030807 US 2002-301499 20021121  
PRIORITY APPLN. INFO.: US 2001-331935P P 20011121  
OTHER SOURCE(S): MARPAT 139:30773

AB Peptides and pharmaceutical compns. comprising them are disclosed.  
Conjugated peptides linked to detectable agents and/or cytotoxic agents.  
are disclosed. A method of detecting tumors that have cell-surface p185  
is disclosed. Methods of preventing transformation of a normal cell into  
a tumor cell in an individual at risk of developing a tumor having tumor  
cells which have p185 on their surfaces are disclosed. Methods of  
treating an individual who has cancer characterized by tumor cells that  
have a p185 on their cell surfaces are disclosed.

IT 75853-32-6

RL: PRP (Properties)  
(unclaimed sequence; peptides that bind to p185, and methods for the  
treatment and diagnosis of tumors)

L5 ANSWER 2 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:849477 HCAPLUS  
DOCUMENT NUMBER: 137:348514  
TITLE: High throughput screening methods using magnetic  
resonance imaging agents  
INVENTOR(S): Meade, Thomas J.  
PATENT ASSIGNEE(S): Metaprobe, Inc., USA  
SOURCE: PCT Int. Appl., 71 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.    | KIND  | DATE     | APPLICATION NO. | DATE     |
|---------------|---|----------|-----------------|----------|
| WO 2002087632 | A1  | 20021107 | WO 2002-US14194 | 20020502 |
| W:            | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,<br>CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,<br>GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,<br>LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,<br>PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,<br>UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |          |                 |          |
| RW:           | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,<br>CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,<br>BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  |          |                 |          |

US 2002197648 A1 20021226 US 2002-139145 20020502  
PRIORITY APPLN. INFO.: US 2001-288963P P 20010502

AB The invention relates to a wide variety of different methods and compns.  
that find use in high throughput screening applications utilizing magnetic  
resonance imaging (MRI) contrast agents. The invention provides a library  
of MRI contrast agents comprising a chelate, a paramagnetic metal ion, and  
a different candidate agent. The candidate agent may be covalently  
attached to the chelate, or indirectly attached to the chelate via a  
linker. Suitable candidate agents include peptides, carbohydrates,  
nucleic acids and lipids. The methods may be applicable for screening for  
protease-activated MRI contrast agents, for screening of animals  
pretreated with a drug candidate, for screening of transgenic animals, for  
imaging gene expression, for imaging disease progression, etc.

IT 75853-32-6

RL: PRP (Properties)  
(unclaimed sequence; high throughput screening methods using magnetic  
resonance imaging agents)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

L5 ANSWER 3 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:234133 HCAPLUS  
DOCUMENT NUMBER: 136:402018  
TITLE: Silyl-Substituted Amino Acids: New Routes to the  
Construction of Selectively Functionalized  
Peptidomimetics  
AUTHOR(S): Sun, Haizhou; Moeller, Kevin D.  
CORPORATE SOURCE: Department of Chemistry, Washington University, St.  
Louis, MO, 63130, USA  
SOURCE: Organic Letters (2002), 4(9), 1547-1550  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 136:402018

AB Silylated amino acids have been incorporated into peptides and then  
converted into N-acyliminium ions with the use of an anodic oxidn.  
reaction. The result is a method for selectively incorporating  
conformational constraints or external nucleophiles within the peptide.

IT 429685-03-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of silylated amino acid building blocks for peptides and their  
conversion into peptidomimetics via anodic oxidn.)

IT 429685-04-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of silylated amino acid building blocks for peptides and their  
conversion into peptidomimetics via anodic oxidn.)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:78410 HCAPLUS  
DOCUMENT NUMBER: 134:147856  
TITLE: Preparation of polypeptide dendrimers as unimolecular  
carriers of diagnostic imaging contrast agents,  
bioactive substances and drugs  
INVENTOR(S): Verdini, Antonio  
PATENT ASSIGNEE(S): Italy  
SOURCE: PCT Int. Appl., 33 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.    | KIND   | DATE     | APPLICATION NO. | DATE     |
|---------------|--|----------|-----------------|----------|
| WO 2001007469 | A2   | 20010201 | WO 2000-EP7022  | 20000721 |
| WO 2001007469 | A3   | 20010510 |                 |          |
| W:            | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |          |                 |          |
| RW:           | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG   |          |                 |          |
| EP 1200461    | A2   | 20020502 | EP 2000-949393  | 20000721 |
| R:            | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL   |          |                 |          |

JP 2003506326 T2 20030218 JP 2001-512552 20000721  
 NZ 517231 A 20030530 NZ 2000-517231 20000721  
 NO 2002000333 A 20020122 NO 2002-333 20020122  
 PRIORITY APPLN. INFO.: IT 1999-FO15 A 19990723  
 WO 2000-EP7022 W 20000721

AB The invention describes new polypeptide dendrimers and processes for their synthesis. The polypeptide dendrimers of the invention have a structure which consists of a multifunctional core moiety from which highly branched polypeptide chains, formed by short peptide branching units, extend radially outwards. The outermost branches surround a lower d. space with hollows and channels into which bioactive substances employed in diagnosis and therapy can be entrapped or covalently linked. The said polypeptide dendrimers are particularly useful in a no. of areas in biol. and medicine as carriers for the delivery of bioactive substances, including drugs, or as carriers of bacterial, viral and parasite antigens, gene-therapy compds. and diagnostic imaging contrast agents. N[CH<sub>2</sub>CH<sub>2</sub>NHCOCH(CH<sub>2</sub>Ph)NH-Gly-Gly-Orn-Gly[Gly-Gly-Orn(Boc)-Gly-Boc]<sub>2</sub>]<sub>3</sub> (Boc = tert-butoxycarbonyl) is an example of a polypeptide dendrimer which was synthesized. Various properties of the polypeptide dendrimers were studied, including stability to enzymic hydrolysis in vitro and immunogenicity in mice and its adjuvant activity when some of the NH<sub>2</sub> groups are covalently linked to the octapeptide antigen Ala-Asn-Pro-Asn-Ala-Asn-Pro-Asn.

IT **323178-52-5P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (prepn. of polypeptide dendrimers as unimol. carriers of diagnostic imaging contrast agents, bioactive substances and drugs)

IT **323178-48-9P 323178-51-4P**

RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of polypeptide dendrimers as unimol. carriers of diagnostic imaging contrast agents, bioactive substances and drugs)

IT **323178-50-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of polypeptide dendrimers as unimol. carriers of diagnostic imaging contrast agents, bioactive substances and drugs)

L5 ANSWER 5 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:314580 HCAPLUS

DOCUMENT NUMBER: 132:326152

TITLE: DDS compounds and method for assaying the same

INVENTOR(S): Susaki, Hiroshi; Inoue, Kazuhiro; Kuga, Hiroshi; Ikeda, Masahiro; Shiose, Yoshinobu; Korenaga, Hiroshi

PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| WO 2000025825   | A1   | 20000511 | WO 1999-JP6016  | 19991029 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |      |          |                 |          |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,   |      |          |                 |          |

DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 9964880 A1 20000522 AU 1999-64880 19991029  
BR 9915198 A 20010814 BR 1999-15198 19991029  
EP 1155702 A1 20011121 EP 1999-952805 19991029

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO

NO 2001002128 A 20010620 NO 2001-2128 20010430  
ZA 2001004214 A 20020114 ZA 2001-4214 20010523

PRIORITY APPLN. INFO.: JP 1998-310130 A 19981030  
JP 1998-329272 A 19981119  
WO 1999-JP6016 W 19991029

AB The invention relates to a method for assaying a DDS compd. contg. a  
saccharide compd.-modified carboxy C1-4 alkyl-dextran polyalc. and a drug  
compd. [DX8951 or doxorubicin] residue bonded to this carboxy C1-4  
alkyl-dextran polyalc., or a DDS compd. wherein a polymer carrier is bonded  
to a drug compd. residue via a spacer contg. 2 to 8 amino acids bonded  
together via peptide bonds, which involves the step of assaying a  
hydrolyzate obtained by treating the DDS compd. with peptidase.

IT **75853-32-6DP**, DX8951 or doxorubicin conjugates with carboxy C1-4  
alkyl-dextran polyalc. and  
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological  
study); PREP (Preparation); USES (Uses)  
(DDS compds. and method for assaying the same)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:96022 HCAPLUS

DOCUMENT NUMBER: 132:156840

TITLE: Pretargeted delivery of biotin derivative diagnostic  
or therapeutic agents.

INVENTOR(S): Gustavson, Linda M.; Theodore, Louis J.; Su, Fu Min;  
Reno, John M.

PATENT ASSIGNEE(S): Neorx Corp., USA

SOURCE: U.S., 65 pp., Cont.-in-part of U.S. Ser. No. 995,381,  
abandoned.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

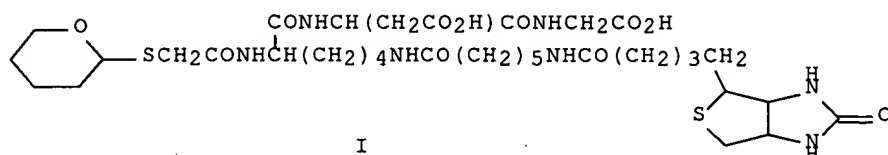
FAMILY ACC. NUM. COUNT: 14

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| US 6022966  | A    | 20000208 | US 1993-156565  | 19931122 |
| US 5283342  | A    | 19940201 | US 1992-895588  | 19920609 |
| WO 9325240  | A2   | 19931223 | WO 1993-US5406  | 19930607 |
| WO 9325240  | A3   | 19940217 |                 |          |
| W: CA, JP, US   |      |          |                 |          |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE    |      |          |                 |          |
| EP 1138334  | A2   | 20011004 | EP 2001-201994  | 19930607 |
| EP 1138334  | A3   | 20020403 |                 |          |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE |      |          |                 |          |
| US 5911969  | A    | 19990615 | US 1994-329617  | 19941026 |
| CA 2177136  | AA   | 19950608 | CA 1994-2177136 | 19941122 |
| WO 9515335  | A2   | 19950608 | WO 1994-US13485 | 19941122 |
| WO 9515335  | A3   | 19950720 |                 |          |
| W: CA, JP   |      |          |                 |          |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE    |      |          |                 |          |
| US 5541287  | A    | 19960730 | US 1994-345811  | 19941122 |
| EP 736035   | A1   | 19961009 | EP 1995-910066  | 19941122 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE |      |          |                 |          |

|                        |    |          |                 |             |
|------------------------|----|----------|-----------------|-------------|
| JP 09505831            | T2 | 19970610 | JP 1995-515670  | 19941122    |
| US 5847121             | A  | 19981208 | US 1995-571816  | 19951213    |
| PRIORITY APPLN. INFO.: |    |          | US 1992-895588  | A2 19920609 |
|                        |    |          | US 1992-995381  | B2 19921223 |
|                        |    |          | WO 1993-US5406  | A2 19930607 |
|                        |    |          | US 1992-995383  | A2 19921223 |
|                        |    |          | EP 1993-915235  | A3 19930607 |
|                        |    |          | US 1993-156565  | A 19931122  |
|                        |    |          | US 1994-345811  | A3 19941122 |
|                        |    |          | WO 1994-US13485 | W 19941122  |

OTHER SOURCE(S): MARPAT 132:156840  
GI



AB Methods, compds., compns. and kits that relate to pretargeted delivery of diagnostic and therapeutic agents are disclosed. In particular, methods for radiometal labeling of biotin, as well as related compds., are described. One example compd. prepd. was I which was complexed with 99mTc or 186Re.

IT **167861-74-7P 180737-55-7P 180737-56-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(pretargeted delivery of biotin deriv. diagnostic or therapeutic agents)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:50615 HCAPLUS

DOCUMENT NUMBER: 133:28087

TITLE: A triglycine linker improves tumor uptake and biodistributions of 67-Cu-Labeled anti-neuroblastoma MAb chCE7 F(ab')<sub>2</sub> fragments

AUTHOR(S): Zimmermann, K.; Gianollini, S.; Schubiger, P. A.; Novak-Hofer, I.

CORPORATE SOURCE: Center for Radiopharmaceutical Sciences, Paul Scherrer Institute, Villigen, Switz.

SOURCE: Nuclear Medicine and Biology (1999), 26(8), 943-950  
CODEN: NMBIEO; ISSN: 0969-8051

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The peptide-linked copper chelators CPTA-triglycyl-l-p-isothiocyanato-phenylalanine (CPTA-R1-NCS) as well as DOTA-triglycyl-l-p-isocyanato-phenylalanine (DOTA-R1-NCS) were synthesized and coupled to F(ab')<sub>2</sub> fragments of the anti-neuroblastoma monoclonal antibody (MAb) chCE7. 67Cu-labeled conjugates were compared with the original CPTA- and DO3A-F(ab')<sub>2</sub> in vitro and in vivo in mice bearing neuroblastoma xenografts. With the CPTA-R1-F(ab')<sub>2</sub>, biodistributions were improved, because radioactivity present in the kidney was reduced. With the DOTA-R1-F(ab')<sub>2</sub>, clearance from the blood was slower and tumor uptake was higher compared with the other conjugates. DOTA-R1-F(ab')<sub>2</sub> achieved the best tumor/tissue ratios.

IT **273944-80-2DP**, 67Cu-labeled MAb conjugate **273944-81-3DP**, 67Cu-labeled MAb conjugate

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(triglycine linker improves tumor uptake and biodistributions of 67-Cu-Labeled anti-neuroblastoma MAb chCE7 F(ab')<sub>2</sub> fragments)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:763905 HCAPLUS

DOCUMENT NUMBER: 132:15631

TITLE: Antitumor or antiinflammatory drug composites

INVENTOR(S): Susaki, Hiroshi; Inoue, Kazuhiro; Kuga, Hiroshi

PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.    | KIND   | DATE     | APPLICATION NO. | DATE     |
|---------------|--|----------|-----------------|----------|
| WO 9961061    | A1   | 19991202 | WO 1999-JP2681  | 19990521 |
| W:            | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |          |                 |          |
| RW:           | GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG   |          |                 |          |
| CA 2333321    | AA   | 19991202 | CA 1999-2333321 | 19990521 |
| AU 9937333    | A1   | 19991213 | AU 1999-37333   | 19990521 |
| EP 1080732    | A1   | 20010307 | EP 1999-919664  | 19990521 |
| R:            | BE, CH, DE, FR, GB, IT, LI, NL, SE   |          |                 |          |
| NO 2000005913 | A  | 20010122 | NO 2000-5913    | 20001122 |

PRIORITY APPLN. INFO.: JP 1998-140915 A 19980522  
WO 1999-JP2681 W 19990521

AB Drug composites useful as DDS compds., which are represented by the general formula: A-R-NH-Y-CH<sub>2</sub>-O-CO-Q (wherein A is a polymer serving as a carrier for a drug; R is a spacer comprising one amino acid mol. or one comprising 2 to 8 amino acid mols. bound to each other through peptide linkage; Y is optionally substituted phenylene; and Q is a residue of a drug compd. such as an antitumor agent). The composites permit the speedy and regioselective release of drug compds. such as antitumor or anti-inflammatory agents, thus exhibiting expected drug effects without fail. A composite of DX-8951 [(1S,9S)-1-Amino-9-ethyl-5-fluoro-2,3-dihydro-9-hydroxy-4-methyl-1H,12H-benzo[de]pyrano[3',4':6,7]indolizino[1,2-b]quinolin-10,13(9H,15H)-dione] was prepd. from DX-8951 methanesulfonic acid salt, dextran polyalc. Na salt, Boc-Gly-Gly-Phe-Gly-OH, 4-aminobenzylalc., and bis(4-nitrophenyl)carbonate.

IT 251459-40-2DP, reaction products with dextran and acetic acid  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(antitumor or antiinflammatory drug dextran polyalc. conjugates)

IT 251459-34-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of antitumor or antiinflammatory drug dextran polyalc. conjugates)

IT 251459-36-6P 251459-38-8P 251459-40-2DP,

reaction products with dextran and acetic acid 251459-42-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of antitumor or antiinflammatory drug dextran polyalc. conjugates)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:698781 HCAPLUS

DOCUMENT NUMBER: 130:106984

TITLE: Comparison of 1,4,7,10-tetraazacyclododecane-N,N',N'',N'''-tetraacetic acid (DOTA)-peptide-ChL6, a novel immunoconjugate with catabolizable linker, to 2-iminothiolane-2-[p-(bromoacetamido)benzyl]-DOTA-ChL6 in breast cancer xenografts

AUTHOR(S): DeNardo, Gerald L.; Kroger, Linda A.; Meares, Claude F.; Richman, Carol M.; Salako, Qansy; Shen, Sui; Lamborn, Kathleen R.; Peterson, James J.; Miers, Laird A.; Zhong, Gao Ren; DeNardo, Sally J.

CORPORATE SOURCE: Department of Internal Medicine, School of Medicine, University of California Davis, Sacramento, CA, 95816, USA

SOURCE: Clinical Cancer Research (1998), 4(10), 2483-2490  
CODEN: CCREF4; ISSN: 1078-0432

PUBLISHER: American Association for Cancer Research

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Radioimmunotherapy using <sup>131</sup>I-ChL6 antibody has shown promise in patients with breast cancer. To enhance this potential, a novel ChL6 immunoconjugate that is catabolizable and tightly binds <sup>90</sup>Y and <sup>111</sup>In was developed. The immunoconjugate, 1,4,7,10-tetraazacyclododecane-N,N',N'',N'''-tetraacetic acid (DOTA)-peptide-ChL6, consists of the macrocyclic chelator DOTA linked to ChL6 by a peptide that is preferentially catabolized in the liver. The pharmacokinetic and dosimetric properties of the radioimmunoconjugates (RICs) <sup>111</sup>In- and <sup>90</sup>Y-DOTA-peptide-ChL6 and <sup>111</sup>In- and <sup>90</sup>Y-2-iminothiolane (2-IT)-2-[p-(bromoacetamido)benzyl]-DOTA-ChL6 were compared in athymic mice bearing HBT3477 human breast cancer xenografts. Each of the RICs was stable in vivo and concd. well in the xenografts. Liver concn., cumulative radioactivity (activity over time), and radiation dose of the DOTA-peptide-ChL6 RICs were one-third to one-half of those of the corresponding 2-IT-2-[p(bromoacetamido)benzyl]-DOTA-ChL6 RICs. Indium-111 RICs were imperfect tracers for corresponding <sup>90</sup>Y RICs, although their pharmacokinetics and radiation dosimetries were similar. The results of this study were consistent with previously published in vitro data, which indicated that the peptide linker of DOTA-peptide-ChL6 was catabolized by cathepsin B. The cumulative activities and radiation doses to the liver of DOTA-peptide-ChL6 RICs were one-half of those of corresponding RICs with the 2-IT linker. Preliminary data from pilot studies in patients with breast cancer are in accord with these observations. These novel DOTA-peptide RICs seem to have excellent clin. potential for radioimmunotherapy assocd. with marrow transplantation, for which liver radiation is likely to be dose limiting for <sup>90</sup>Y.

IT 219721-93-4D, radioimmunoconjugate with DOTA and ChL6 antibody

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(comparison of 1,4,7,10-tetraazacyclododecane-N,N',N'',N'''-tetraacetic acid (DOTA)-peptide-ChL6 to 2-iminothiolane-2-[p-(bromoacetamido)benzyl]-DOTA-ChL6 in breast cancer xenografts)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L5 ANSWER 10 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:164839 HCAPLUS  
DOCUMENT NUMBER: 126:141273  
TITLE: Carbonic Anhydrase-Inhibitor Binding: From Solution to the Gas Phase  
AUTHOR(S): Wu, Qinyuan; Gao, Jinming; Joseph-McCarthy, Diane; Sigal, George B.; Bruce, James E.; Whitesides, George M.; Smith, Richard D.  
CORPORATE SOURCE: Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA, 99352, USA  
SOURCE: Journal of the American Chemical Society (1997), 119(5), 1157-1158  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The binding of para-substituted benzenesulfonamide inhibitors to bovine carbonic anhydrase II (BCAII, EC 4.2.1.1) in the gas phase and in soln. has been studied by electrospray ionization-mass spectrometry and fluorescence spectroscopy, resp. The off-rates of BCAII-inhibitor complexes in soln. are primarily detd. by the hydrophobic interactions between the inhibitor and the enzyme, while their corresponding gas phase stabilities are governed by the polar surface interactions. The results provide insights into the factors governing gas phase stability of the charged complexes, and show that relative stabilities in soln. and the gas phase are substantially different.

IT 176171-19-0

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)  
(carbonic anhydrase-inhibitor binding in soln. and gas phase)

L5 ANSWER 11 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:494751 HCAPLUS  
DOCUMENT NUMBER: 125:204516  
TITLE: Diagnostic and therapeutic pretargeting methods using metal chelates  
INVENTOR(S): Yau, Eric K.; Theodore, Louis J.; Gustavson, Linda M.  
PATENT ASSIGNEE(S): Neorx Corporation, USA  
SOURCE: U.S., 68 pp., Cont.-in-part of U.S. Ser. No. 156,565, abandoned.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 14  
PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE        |
|---|------|----------|-----------------|-------------|
| US 5541287  | A    | 19960730 | US 1994-345811  | 19941122    |
| US 5283342  | A    | 19940201 | US 1992-895588  | 19920609    |
| EP 1138334  | A2   | 20011004 | EP 2001-201994  | 19930607    |
| EP 1138334  | A3   | 20020403 |                 |             |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE |      |          |                 |             |
| US 6022966  | A    | 20000208 | US 1993-156565  | 19931122    |
| US 5911969  | A    | 19990615 | US 1994-329617  | 19941026    |
| US 5847121  | A    | 19981208 | US 1995-571816  | 19951213    |
| PRIORITY APPLN. INFO.:  |      |          |                 |             |
|   |      |          | US 1992-895588  | A2 19920609 |
|   |      |          | US 1992-995381  | B2 19921223 |
|   |      |          | US 1993-156565  | B2 19931122 |
|   |      |          | US 1992-995383  | A 19921223  |
|   |      |          | EP 1993-915235  | A3 19930607 |

OTHER SOURCE(S): CASREACT 125:204516; MARPAT 125:204516

AB Methods, compds., compns., and kits that relate to pretargeted delivery of diagnostic (e.g. imaging) and therapeutic agents are disclosed. A targeting moiety-antiligand conjugate is administered in vivo; upon target localization of this conjugate (pretargeting) and clearance of the conjugate from the circulation, an active agent-ligand conjugate is parenterally administered. Alternatively, a targeting moiety-ligand conjugate is administered in vivo; upon target localization and clearance of the conjugate from the circulation, an active agent-antiligand conjugate is parenterally administered. A preferred ligand-antiligand pair is biotin and avidin. Preferred targeting moieties are antibodies, antibody fragments, peptides, hormones, oligonucleotides, and cell surface receptor proteins. Preferred active agents are toxins, antitumor agents, drugs, and radionuclides. In particular, methods for prodn. of low-mol.-wt. radioiodinated biotin derivs., and for radiometal labeling of biotin and related compds. with <sup>99m</sup>Tc, <sup>186</sup>Re, and <sup>188</sup>Re by conjugation with a metal-chelating moiety are described. Thus, p-aminobenzyl-1,4,7,10-tetraazacyclododecane-N,N',N'',N'''-tetraacetic acid (I) was prepd. in several steps from N-tert-butoxycarbonylglycine p-nitrophenyl ester, ethylenediamine, and N-iodoacetyl-p-nitrophenylalanine using benzotriazolyloxytris(dimethylamino)phosphonium hexafluorophosphate for cyclocondensation; I was then coupled with N-biotinyl-N-methylglycine and complexed with 90Y. The chelate and its sulfoxide radiolysis product bound to avidin.

IT **167861-61-2P 167861-62-3P 167861-74-7P**  
**180737-51-3P 180737-55-7P 180737-56-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(diagnostic and therapeutic pretargeting methods using metal chelates)

L5 ANSWER 12 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:158255 HCAPLUS

DOCUMENT NUMBER: 124:317848

TITLE: Benzenesulfonamide-peptide conjugates as probes for secondary binding sites near the active site of carbonic anhydrase

AUTHOR(S): Sigal, George B.; Whitesides, George M.

CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(5), 559-64

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Libraries of N-(4-sulfamoylbenzoyl)oligoglycines terminated with different L-amino acids were screened to identify tight binding inhibitors of human carbonic anhydrase II. Inhibitors terminated with hydrophobic amino acids showed significant enhancements in binding compared to the corresponding glycine derivs. No enhancements were obsd. due to polar interactions.

IT **165682-42-8P 176171-07-6P 176171-17-8P**  
**176171-18-9P 176171-19-0P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and carbonic anhydrase active site binding of benzenesulfonamide-peptide conjugates)

L5 ANSWER 13 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:795164 HCAPLUS

DOCUMENT NUMBER: 123:225940

TITLE: Pretargeting methods and compounds comprising

radiometal labeled biotin and biotin- or streptavidin-antibody conjugates

\*INVENTOR(S): Yau, Eric K.; Theodore, Louis J.; Gustavson, Linda M.

PATENT ASSIGNEE(S): Neorx Corp., USA

SOURCE: PCT Int. Appl., 180 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 14

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE        |
|---|------|----------|-----------------|-------------|
| WO 9515335  | A2   | 19950608 | WO 1994-US13485 | 19941122    |
| WO 9515335  | A3   | 19950720 |                 |             |
| W: CA, JP   |      |          |                 |             |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE    |      |          |                 |             |
| US 6022966  | A    | 20000208 | US 1993-156565  | 19931122    |
| EP 736035   | A1   | 19961009 | EP 1995-910066  | 19941122    |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE |      |          |                 |             |
| JP 09505831   | T2   | 19970610 | JP 1995-515670  | 19941122    |
| PRIORITY APPLN. INFO.:  |      |          |                 |             |
|   |      |          | US 1993-156565  | A 19931122  |
|   |      |          | US 1992-895588  | A2 19920609 |
|   |      |          | US 1992-995381  | B2 19921223 |
|   |      |          | WO 1993-US5406  | A2 19930607 |
|   |      |          | WO 1994-US13485 | W 19941122  |

AB Methods, compds., compns. and kits that relate to pretargeted delivery of diagnostic and therapeutic agents are disclosed. In particular, methods for radiometal labeling of biotin, as well as related compds., are described. Articles of manuf. useful in pretargeting methods are also discussed. In example, 186Re-chelated biotin and biotinylated monoclonal antibody to human colon tumor (NR-LU-10) were prep'd. and used in combination with avidin were performed in a 3-step pretargeting protocol in nude mice implanted with human colon tumor xenografts, and a enhanced tumor uptake of 186Re-chelated biotin in the presence of biotinylated antibody and avidin was obs'd. Also, streptavidin-NR-LU-10 conjugates were prep'd. and used in combination with 186Re-chelated biotin and asialoorosomucoid clearing agent (prepn. described) for two-step pretargeting protocol expt.

IT **167861-61-2P 167861-62-3P 167861-63-4P**  
**167861-64-5P 167861-74-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(radiometal-labeled biotin and conjugates of antibody and biotin or streptavidin in pretargeting method for tumor diagnosis and therapy)

L5 ANSWER 14 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:578931 HCAPLUS

DOCUMENT NUMBER: 123:106470

TITLE: Molecular Dynamics Simulations of  
H2NSO2C6H4CONH(Gly)3OBn Bound to the Active Site of  
Human Carbonic Anhydrase II

AUTHOR(S): Chin, Donovan N.; Whitesides, George M.

CORPORATE SOURCE: Department of Chemistry, Harvard University,  
Cambridge, MA, 02138, USA

SOURCE: Journal of the American Chemical Society (1995),  
117(23), 6153-64

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper describes stochastic boundary mol. dynamics simulations of a benzyl-terminated oligoglycine inhibitor, H2NSO2C6H4CO(NHCH2CO)3R (SG3Bn),

bound to the active site of human carbonic anhydrase II (HCAII, EC 4.2.1.1) in the presence of water. The position of the terminal benzyloxy group ( $R = \text{OCH}_2\text{C}_6\text{H}_5$ ) was not defined in a crystal structure of this complex. The simulation suggested that the benzyl group assocd. with the hydrophobic residues Phe-20 and Pro-202 and that this assocn. accounted for the decrease in the value of  $K_d$  obsd. for this benzyl-terminated inhibitor relative to other inhibitors with hydrophilic terminal groups. The av. conformation obsd. for the oligoglycines in the inhibitor from the simulation was significantly different from the conformation inferred in the crystal structure. For example, the simulation indicated that the .PSI. angle of Gly-1 and the .PHI. angle of Gly-2 shifted by about 50.degree. from their values in the crystal structure within the first 2.5 ps of the 150 ps simulation. The simulation suggested that the calcd. av. conformation of the oligoglycines in the inhibitor-in its bound state with the protein-was a result of (1) the formation of hydrogen bonds with the surrounding mols. of water (these were included in the simulation) and (2) an accompanying improvement of .pi.-face assocns. with the hydrophobic wall of the protein. These results, and their implications for the design of new inhibitors, are discussed.

IT **165682-42-8**

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)  
(mol. dynamics simulations of  $\text{H}_2\text{NSO}_2\text{C}_6\text{H}_4\text{CONH}(\text{Gly})_3\text{OBn}$  bound to active site of human carbonic anhydrase II)

L5 ANSWER 15 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:490207 HCAPLUS

DOCUMENT NUMBER: 119:90207

TITLE: Synthesis, metal chelate stability studies, and enzyme digestion of a peptide-linked DOTA derivative and its corresponding radiolabeled immunoconjugates

AUTHOR(S): Li, Min; Meares, Claude F.

CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616-0935, USA

SOURCE: Bioconjugate Chemistry (1993), 4(4), 275-83

CODEN: BCCHES; ISSN: 1043-1802

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By directly coupling a tetrapeptide to DOTA through an amide bond, a novel DOTA deriv., DOTA-glycylglycylglycyl-L-p-nitrophenylalanine amide, was synthesized. This new precursor bifunctional chelating agent was converted to DOTA-glycylglycylglycyl-L-p-isothiocyanatophenylalanine and conjugated to monoclonal antibody Lym-1. Serum stability studies show that the radiolabeled conjugates are kinetically inert under physiol. conditions. The rates of loss of radiometals in human serum are 0.1% per day for  $\text{In}^{3+}$ , 0.02% per day for Y3, and 0.3% per day for  $\text{Cu}^{2+}$ -labeled immunoconjugates. In the presence of the liver enzyme cathepsin B, an in vitro digestion of 114mIn-labeled conjugate yields a small fragment contg. 114mIn. Characterization of the cleavage products shows that this liver enzyme hydrolyzes the peptide linkage before the phenylalanine residue, freeing the In-DOTA-triglycine complex from the conjugate. However, the liver enzyme cathepsin D does not cleave the linkage over the span of 7 days.

IT **149226-84-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and coupling with DOTA)

IT **149206-85-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and trifluoroacetylation of)

L5 ANSWER 16 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:470314 HCAPLUS

DOCUMENT NUMBER: 117:70314  
TITLE: Simultaneous use of 1-hydroxybenzotriazole and copper(II) chloride as additives for racemization-free and efficient peptide synthesis by the carbodiimide method  
AUTHOR(S): Miyazawa, Toshifumi; Otomatsu, Toshihiko; Fukui, Yoshimasa; Yamada, Takashi; Kuwata, Shigeru  
CORPORATE SOURCE: Fac. Sci., Konan Univ., Kobe, Japan  
SOURCE: International Journal of Peptide & Protein Research (1992), 39(4), 308-14  
CODEN: IJPPC3; ISSN: 0367-8377

DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 117:70314

AB In the carbodiimide mediated coupling of PhCH<sub>2</sub>O<sub>2</sub>C-Gly-L-Val-OH with H-L-Val-OMe in DMF, the simultaneous use of 1-hydroxybenzotriazole (HOBt) and copper(II) chloride as additives was found to give the desired peptide in a high yield without racemization. In the presence of HOBt, reducing the amt. of copper(II) chloride produced a higher yield. Besides improving the coupling efficiency as compared with the case using copper(II) chloride alone as an additive, the present procedure offered another advantage for racemization suppression. Thus, even for the couplings where a low level of racemization was obsd. in the presence of copper(II) chloride, the simultaneous addn. of HOBt and copper(II) chloride resulted in the elimination of racemization. The effectiveness of this new procedure using the two carbodiimide additives in the synthesis of biol. active peptides was assessed by the prepn. of a protected leucine-enkephalin. In the 4 + 1 segment condensation using HOBt and copper(II) chloride simultaneously as additives, no racemization was detected and the yield was high enough. The elimination of racemization and improvement of coupling efficiency produced by the present procedure can be attributable to a reduced tendency for the activated forms of the carboxyl component to form a 5(4H)-oxazolone by the action of HOBt, and to the prevention of racemization by copper(II) chloride of the small amt. of the oxazolone formed which is not eliminated by the action of HOBt alone.

IT **24848-63-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and peptide coupling of, with leucine ester, effect of hydroxybenzotriazole and cupric chloride on racemization in)

L5 ANSWER 17 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:17641 HCAPLUS  
DOCUMENT NUMBER: 116:17641  
TITLE: The specificity of chymotrypsin. A statistical analysis of hydrolysis data  
AUTHOR(S): Schellenberger, Volker; Braune, Katrin; Hofmann, Hans Joerg; Jakubke, Hans Dieter  
CORPORATE SOURCE: Sect. Biowiss., Univ. Leipzig, Leipzig, O-7010, Germany  
SOURCE: European Journal of Biochemistry (1991), 199(3), 623-36  
CODEN: EJBCAI; ISSN: 0014-2956  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB From the literature all available quant. data on the chymotrypsin-catalyzed hydrolysis of a series of amino acid and peptide substrates were collected. Utilizing this data base, calcns. were performed on their quant. structure/activity relationship (QSAR). The substrates were considered to be composed of fragments; log(kcat/Km) values for the substrates resulted from additive contribution of their fragments. Despite the fact that the kinetic consts. in the data base were detd. by

different authors under various reaction conditions, the data are well described by the simple additivity model. Obviously, the intrinsic specificity of chymotrypsin dominates the influence of varying reaction conditions.

IT 78682-74-3 135612-66-7

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)

(reaction of, with chymotrypsin, quant. structure-activity relationship study of)

L5 ANSWER 18 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:240639 HCAPLUS

DOCUMENT NUMBER: 114:240639

TITLE: Preparation and activity of controlled-action anesthetic compounds and pharmaceutical compositions containing them

INVENTOR(S): Raynal, Serge; Grousset, Maryse; Rancurel, Alain

PATENT ASSIGNEE(S): Societe Nationale des Poudres et Explosifs, Fr.; Laboratoires Pharmascience

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.   | KIND | DATE     | APPLICATION NO. | DATE     |
|--|------|----------|-----------------|----------|
| WO 9011292   | A2   | 19901004 | WO 1990-FR197   | 19900323 |
| WO 9011292   | A3   | 19901115 |                 |          |
| W: JP, US  |      |          |                 |          |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE |      |          |                 |          |
| FR 2644697   | A1   | 19900928 | FR 1989-3909    | 19890324 |
| FR 2644697   | B1   | 19920515 |                 |          |
| EP 418365  | A1   | 19910327 | EP 1990-905561  | 19900323 |

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE

PRIORITY APPLN. INFO.: FR 1989-3909 19890324

WO 1990-FR197 19900323

OTHER SOURCE(S): CASREACT 114:240639; MARPAT 114:240639

AB The title compds. are (poly)amino acid derivs. of aminobenzoic acid-derived anesthetics, i.e. (AA)nN(R)B [B is such that RNHB is an aminobenzoic acid-derived anesthetic; R = H, (un)substituted C1-5 alkyl; AA = .alpha.-amino acid; n = 1-10; with provisions] and their pharmaceutically acceptable salts. Thus, tert-butoxycarbonylalanine (BOC-Ala) was reacted with N-methylmorpholine and isopropenyl chloroformate, and the anhydride formed was further reacted with benzocaine to form BOC-Ala-benzocaine, which was later N-deprotected. In animal tests, when NH2(Gly)p-Phe-benzocaine (I) (p = 0-4) was injected at a molar concn. equiv. to 1% benzocaine, I (p = 0-2) allowed lengthy anesthesia (5-6 h); for I (p = 3, 4), anesthetic activity was const. for 3 h, then abruptly dropped by 50% (i.e. half of the test animals were no longer anesthetized) in 30 min and disappeared totally in 1-1.5 h. When glycine was replaced by alanine in I, similar results were obtained.

IT 133954-78-6

RL: BIOL (Biological study)  
(controlled-action anesthetic)

IT 134002-70-3

RL: BIOL (Biological study)  
(for controlled-action conduction anesthetic)

L5 ANSWER 19 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:192393 HCAPLUS

DOCUMENT NUMBER: 114:192393  
TITLE: Release of p-nitroaniline from oligopeptide side chains attached to N-(2-hydroxypropyl)methacrylamide copolymers during incubation with rat intestinal brush border enzymes  
AUTHOR(S): Kopeckova, Pavla; Longer, Mark A.; Woodley, John F.; Duncan, Ruth; Kopecek, Jindrich  
CORPORATE SOURCE: Dep. Pharm., Univ. Utah, Salt Lake City, UT, 84112, USA  
SOURCE: Makromolekulare Chemie, Rapid Communications (1991), 12(2), 101-6  
CODEN: MCRCD4; ISSN: 0173-2803  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Rat intestinal brush border enzymes cleaved a terminal p-nitroaniline (NAP) residue from oligopeptide side chains attached to HEMA copolymers. The rate of release showed an approx. 10-fold variation depending on the amino acid compn. and length of the side chain. Longer side chains showed faster rates of NAP release. The results were discussed in terms of designing macromol. drugs which would be activated specifically by brush border membrane enzymes at the mucosal surface and at the same time being resistant to the hydrolysis by laminal enzymes.  
IT **61435-98-1**  
RL: BIOL (Biological study)  
(nitroaniline release from, on incubation with intestinal brush border enzymes)

L5 ANSWER 20 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1990:441278 HCAPLUS  
DOCUMENT NUMBER: 113:41278  
TITLE: Gly-L-Phe-OMe, a useful derivatization reagent for chiral separation of N-(benzyloxycarbonyl) amino acids by reversed-phase high-performance liquid chromatography  
AUTHOR(S): Yamada, Takashi; Dejima, Koichi; Shimamura, Masao; Miyazawa, Toshifumi; Kuwata, Shigeru  
CORPORATE SOURCE: Fac. Sci., Konan Univ., Kobe, 658, Japan  
SOURCE: Chemistry Express (1989), 4(11), 725-8  
CODEN: CHEXEU; ISSN: 0911-9566  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 113:41278  
AB Gly-L-Phe-OMe has been found to be a useful derivatization reagent for chiral sepn. of N-(benzyloxycarbonyl) amino acids and, thus, of amino acids themselves by reversed-phase HPLC.  
IT **47458-92-4**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(peptide coupling of, with DL-valine deriv.)

L5 ANSWER 21 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1990:3104 HCAPLUS  
DOCUMENT NUMBER: 112:3104  
TITLE: Kinetic analysis of the carboxypeptidase. A hydrolysis of oligopeptides by reversed-phase high-performance liquid chromatography  
AUTHOR(S): Serra, M. A.; Aviles, F. X.; Giralt, E.; Cuchillo, C. M.  
CORPORATE SOURCE: Fac. Cienc., Univ. Auton. Barcelona, Barcelona, 08193, Spain  
SOURCE: Journal of Chromatography (1989), 479(1), 27-37  
CODEN: JOCRAM; ISSN: 0021-9673  
DOCUMENT TYPE: Journal  
LANGUAGE: English

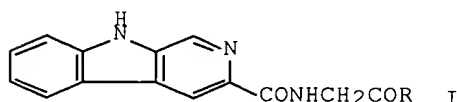
AB A reversed-phase HPLC-based method was developed to follow the time course of the hydrolytic action of pancreatic carboxypeptidase A on oligopeptide substrates of the general formula, benzoyl(glycyl)n-L-phenylalanine, n being in the range 1-5. The proposed procedure was sensitive at the nanomolar level of substrate, but also allowed the kinetics of substrate hydrolysis to be investigated over a wide range of concns. The prior quenching of the carboxypeptidase activity and the use of isocratic conditions for the rapid sepn. of the substrates and their products (in <8 min for the slowest one), allowed the automation of the procedure, which could become an easy and versatile alternative to the commonly used spectrophotometric methods. A comparative evaluation of the use of a spectrophotometric method to measure carboxypeptidase A activity on the same substrates indicated that the latter was not valid for long oligopeptides (n .gtoreq. 2) at concns. of >5 mM owing to an interference of a physicochem. nature. For benzoylglycyl-L-phenylalanine (n = 1), the apparent kinetic parameters were calcd. by means of the HPLC method and by a well established spectrophotometric procedure, and both yielded similar values.

IT **58688-92-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L5 ANSWER 22 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1987:598895 HCAPLUS  
DOCUMENT NUMBER: 107:198895  
TITLE: Oligopeptides of .beta.-carboline-3-carboxylic acid.  
Synthesis and benzodiazepine receptor affinity  
AUTHOR(S): Lippke, Klaus Peter; Mueller, Walter E.; Schunack,  
Walter  
CORPORATE SOURCE: Inst. Pharm., Johannes Gutenberg-Univ., Mainz, D-6500,  
Fed. Rep. Ger.  
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1987),  
320(2), 145-53  
CODEN: ARPMAS; ISSN: 0365-6233  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 107:198895  
GI



AB The title compds., e.g., I [R = NHCH2CO2Et, (S)-NHCH(CO2Me)CH2OH, (S)-NHCHMeCO2Me, NHCH2CH2OH], were prepd. and tested for their affinity for the benzodiazepine receptor in mouse brain membranes. Structure activity relationships were detd. Thus, I (R = OH), prepd. from .beta.-carboline-3-carboxylic acid and H2NCH2CO2Me, was treated with H2NCH2CO2Et in DMF contg. carbonyldiimidazole to give I (R = NHCH2CO2Et).

IT **110672-90-7P**

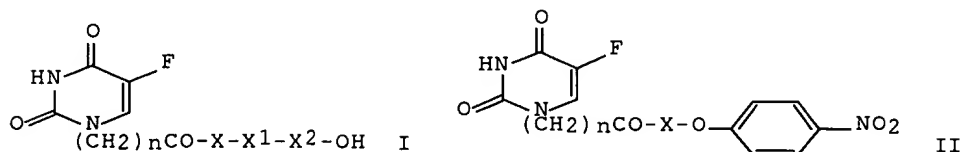
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and benzodiazepine receptor affinity of)

L5 ANSWER 23 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1986:573025 HCAPLUS  
DOCUMENT NUMBER: 105:173025  
TITLE: Synthesis and antitumor activities of 5-fluorouracil  
oligopeptides  
AUTHOR(S): Zhuo, Renxi; Fan, Changlie; Zhao, Rulin



CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Wuhan, Peop. Rep. China  
 SOURCE: Youji Huaxue (1986), (2), 121-5  
 CODEN: YCHHDX; ISSN: 0253-2786  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 OTHER SOURCE(S): CASREACT 105:173025  
 GI



AB 5-Fluorouracil dipeptides I ( $n = 1, 2, X = \text{null}, X_1-X_2 = \text{Gly-Gly, Gly-Phe}; n = 1, X = \text{null}, X-X_1 = \text{Gly-Leu}$ ) were prepd. by coupling active ester II ( $n = 1 \text{ or } 2, X = \text{null}$ ) with the appropriate dipeptides H- $X_1-X_2-OH$  in NaOH aq. soln. 5-Fluorouracil tripeptides I ( $n = 1, X-X_1-X_2 = \text{Gly-Gly-Phe, Val-Gly-Phe, Val-Leu-Gly}; n = 2, X-X_1-X_2 = \text{Phe-Ala-Gly}$ ) were prepd. by coupling II ( $n, X = \text{same}$ ) with the appropriate dipeptides H- $X_1-X_2-OH$ . I ( $n = 1, X-X_1-X_2 = \text{Gly-Gly-Phe, Val-Leu-Gly}; n = 2, X = \text{null}, X_1-X_2 = \text{Gly-Phe}$ ) showed antitumor activities against Ehrlich ascites carcinoma in mice.

IT 104724-44-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (prepn. and antitumor activity of)

L5 ANSWER 24 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1986:6163 HCAPLUS

DOCUMENT NUMBER: 104:6163

TITLE: Racemization-suppressing effect of copper(II) chloride as a new additive in peptide synthesis by the carbodiimide method; application to the synthesis of Leu-enkephalin

AUTHOR(S): Miyazawa, Toshifumi; Otomatsu, Toshihiko; Fukui, Yoshimasa; Yamada, Takashi; Kuwata, Shigeru

CORPORATE SOURCE: Fac. Sci., Konan Univ., Kobe, 658, Japan  
 SOURCE: Peptide Chemistry (1985), Volume Date 1984, 22nd, 265-70

CODEN: PECHDP; ISSN: 0388-3698

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effects of  $CuCl_2$  on the suppression of racemization in peptide coupling mediated by  $Me_2N(CH_2)_3N:C:NEt$  (I) in the presence or absence of 1-hydroxybenzotriazole (HOBt) were evaluated. No racemization occurred in the coupling of  $PhCH_2O_2C-Gly-L-Val-OH$  with H-Val-OMe by I with the addn. of .gtoreq.0.5 equiv of  $CuCl_2$ ; the yield was better than that by the DCC/ $CuCl_2$  method, but it was low when compared to the I/HOBt method. The desired peptide was obtained in good yield without racemization when 1 equiv. each of  $CuCl$ , and HOBt were added to the I-mediated coupling. The addn. of  $CuCl_2$  was applied to the synthesis of Leu-enkephalin. Thus, the I-mediated coupling of  $Me_3CO_2C-Tyr(CH_2Ph)-Gly-Gly-Phe-OH$  with H-Leu-OMe in the presence of  $CuCl_2$  produced a low level of the undesired epimer, but racemization-free peptide was obtained in good yield when  $CuCl_2$  and HOBt were used simultaneously.

IT 24848-63-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (peptide coupling of, with leucine Me ester by carbodiimide method,

racemization suppression by copper chloride in)

L5 ANSWER 25 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1984:412062 HCAPLUS  
DOCUMENT NUMBER: 101:12062  
TITLE: Enzymic cleavage of side chains of soluble polymers  
AUTHOR(S): Labsky, Jiri; Mikes, Frantisek  
CORPORATE SOURCE: VSCHT, Prague, Czech.  
SOURCE: Sbornik Vysoke Skoly Chemicko-Technologicke v Praze,  
S: Polymery--Chemie, Vlastnosti a Zpracovani (1983),  
S 9, 279-308  
CODEN: SVSZD5; ISSN: 0139-908X  
DOCUMENT TYPE: Journal  
LANGUAGE: Czech

AB Models were prepd. for the study of release rates of biol. active substances (drugs, hormones, inhibitors, or enzymes) covalently bound to sol. org. polymers after endocytosis and exposure to liposomal hydrolases. Sol. polymers, polymethacrylates or poly(hydroxypropylmethacrylamides) with d.p. 25-30, bound by amide bonds with L-phenylalanyl nitroanilides through spacers of variable length and structure (peptides or aliph. chains) were used as carriers. Chymotrypsin [9004-07-3]-catalyzed hydrolysis rates of the C-terminal anilide bonds were correlated with the length and structure of the spacers and the structure of the anilide groups. Steric conditions for the interactions of the spacer chains with chymotrypsin active site and affinity site are discussed.

IT **61435-98-1P 90409-74-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and chymotrypsin hydrolysis of, biomols. and drug release in relation to)

L5 ANSWER 26 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1983:139670 HCAPLUS  
DOCUMENT NUMBER: 98:139670  
TITLE: Cryokinetic studies of the intermediates in the mechanism of carboxypeptidase A  
AUTHOR(S): Galdes, Alphonse; Auld, David S.; Vallee, Bert L.  
CORPORATE SOURCE: Cent. Biochem. Biophys. Sci. Med., Harvard Med. Sch., Boston, MA, 02115, USA  
SOURCE: Biochemistry (1983), 22(8), 1888-93  
CODEN: BICHAW; ISSN: 0006-2960  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The detection and definition of intermediates in reaction pathways, a problem central to delineation of structure-function relations in enzymol., have in general resisted soln. An approach capable of wide application to such studies was developed by employing a combination of cryokinetics and cryospectroscopy as exemplified here by use of carboxypeptidase A. These studies are performed with a low-temp. stopped-flow instrument which also serves as a cryospectrometer. The intermediates are monitored directly through fluorescence generated by radiationless enzyme transfer (RET) between enzyme tryptophans and the dansyl group of enzyme-bound substrate. N-dansylated oligopeptides and their ester analogs exhibit Michaelis-Menten kinetics over the temp. range -20 to +20.degree. with  $k_{cat}/K_m$  values of (1-3)  $\times 10^7$  M<sup>-1</sup> s<sup>-1</sup> at 20.degree., pH 7.5, and the cryosolvent, aq. 4.5M NaCl, does not alter catalysis. There is no chem. evidence of a covalent acyl-enzyme intermediate for any of the peptide or ester substrates studied. However, concurrent cryospectroscopy shows that peptides and esters form metal-bound intermediates whose spectra differ strikingly from one another and from that of the enzyme alone. The cryokinetic data demonstrate for the 1st time the existence of 2 intermediates during the hydrolysis of both peptides and esters. At -20.degree., the formation, interconversion,

and breakdown of these intermediates results in 3 distinct fluorescence steps during substrate hydrolysis: (1) a rapid increase in signal intensity reflects the formation of the Michaelis complex, ES1, in <15 ms; (2) a slower exponential increase in signal intensity signifies the formation of a 2nd hitherto unknown intermediate, ES2; (3) a slow decrease in signal intensity reflects sepn. of the dansyl product from the enzyme. All rate and equil. consts. for the reaction scheme,  $E + S \xrightarrow{\text{dblarw. ES1}} \text{dblarw. ES2} \xrightarrow{\text{fwdarw. E + P}}$ , were detd. The reversible interconversion of ES1 and ES2 shows that the C-terminal product is not liberated prior to the rate-limiting step, and hence, deacylation cannot be rate-limiting. The cryokinetic studies in conjunction with the chem. evidence demonstrate that there is no acyl intermediate in either ester or peptide hydrolysis. The present cryokinetics and the concurrent cyrospectroscopy show that peptides and esters form different metal-bound intermediates and that these 2 types of substrates are hydrolyzed through different mechanisms.

IT **37923-00-5**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with carboxypeptidase A at subzero temp., kinetics of)

L5 ANSWER 27 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1983:107729 HCAPLUS

DOCUMENT NUMBER: 98:107729

TITLE: Glycosyl esters of amino acids. Part XIV. Peptide bond formation by intermolecular aminolysis of D-glucopyranosyl esters of amino acids

AUTHOR(S): Horvat, Stefica; Keglevic, Dina

CORPORATE SOURCE: Dep. Org. Chem. Biochem., "Rudjer Boskovic" Inst., Zagreb, 41001, Yugoslavia

SOURCE: Carbohydrate Research (1982), 108(1), 89-96

CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction of hydroxy (un)protected D-glucopyranosyl esters of N-acyl amino acids with glycine and DL-phenylalanine Me esters in DMF at 37.degree. and dichloromethane at 40.degree., resp., led to rupture of the C-1 ester bond and formation of the corresponding N-acyl dipeptide Me ester. The relative reactivity of the C-1 ester bond toward aminolysis was greatly influenced by the structure of the amino acid nucleophile, the nature of the aglycon side-chain group, and the anomeric configuration of the D-glucopyranosyl ester involved. Evidence for a substantially lower acylating efficiency of the ester at C-2, as compared to that at C-1, was obtained by aminolysis of two fully acetylated 2-O-(acylaminoacyl)-.beta.-D-glucopyranoses. Treatment of 1-O-(glycylglycylglycyl)-.beta.-D-glucopyranose with DL-phenylalanine Me ester in DMF led to parallel hydrolysis and intermol. aminolysis, to give the tripeptide and tetrapeptide Me ester.

IT **84814-48-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

IT **84814-47-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by aminolysis of acyl amino acid glucopyranosyl ester with amino acid Me ester)

L5 ANSWER 28 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1981:476069 HCAPLUS

DOCUMENT NUMBER: 95:76069

TITLE: The kinetics of hydrolysis of some extended N-aminoacyl-L-phenylalanine methyl esters by bovine chymotrypsin A.alpha.. Evidence for enzyme subsite S5

AUTHOR(S): Hill, Christopher R.; Tomalin, Geoffrey

CORPORATE SOURCE: Dep. Biochem., Victoria Univ. Manchester, Manchester, M13 9PL, UK

SOURCE: Biochimica et Biophysica Acta (1981), 660(1), 65-72  
CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A series of N-acetylated peptide Me esters of general formula  
N-acetyl-(glycyl)n-L-phenylalanine Me ester (n = 0-3) was synthesized to  
study the effect of varying aminoacyl chain length on the efficiency of  
chymotrypsin A.alpha. (EC 3.4.21.1) catalyzed ester hydrolysis. Values of  
kcat and Km for each substrate were obtained from kinetic measurements at  
pH 8.00 and 25.0.degree.. For the 1st 3 members of the series (n = 0-2)  
there is an increase in kcat value as the aminoacyl chain length is  
increased. However, the kinetic consts. for the 3rd (n = 2) and 4th (n =  
3) members of the series were very similar. These results are consistent  
with a substrate binding scheme proposed for the isomeric enzyme  
chymotrypsin A.gamma.. The enzyme-catalyzed reactions were also  
investigated over a range of temp. (15-35.degree.). In each case the  
Arrhenius law was obeyed, within exptl. error, and evaluation of  
meaningful values for the thermodyn. functions of activation  
(.DELTA.H.thermod. and .DELTA.S.thermod.) was possible with certain  
assumptions. In contrast to the similarity of kinetic consts. found for  
the 3rd and 4th members of the substrate series, the corresponding values  
of .DELTA.H.thermod. and .DELTA.S.thermod. were markedly different. These  
results, together with those for the 1st 2 members of the series are  
interpreted in terms of a model binding system which is consistent with  
the existence of further enzyme subsites in the S4-S5 region.

IT **33374-78-6P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and deprotection of)

IT **78682-72-1P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and peptide coupling reaction of)

IT **78682-74-3**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with chymotrypsin A.alpha., kinetics of)

L5 ANSWER 29 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1981:1489 HCAPLUS  
DOCUMENT NUMBER: 94:1489  
TITLE: Influence of structural changes in small peptides on  
their inhibition of papain  
AUTHOR(S): Ackerman, Louis G. J.; Pretorius, Helena E.; Van Wyk,  
Pieter J.; Vogelzang, Marion E.  
CORPORATE SOURCE: Natl. Food Res. Inst., CSIR, Pretoria, 0001, S. Afr.  
SOURCE: South African Journal of Chemistry (1980), 33(3), 95-9  
CODEN: SAJCDG; ISSN: 0379-4350  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Several peptides and peptide derivs. were synthesized and their inhibition  
towards papain detd. From the amino acid sequence of the peptides which  
act as inhibitors, a further hydrophobic interaction point in the active  
center is postulated.

IT **75853-32-6**  
RL: BIOL (Biological study)  
(papain inhibition by, active site structure in relation to)

L5 ANSWER 30 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1980:617111 HCAPLUS  
DOCUMENT NUMBER: 93:217111  
TITLE: Aeromonas neutral protease: specificity toward  
extended substrates  
AUTHOR(S): Bayliss, Mary E.; Wilkes, Stella H.; Prescott, John M.

CORPORATE SOURCE: Dep. Biochem. Biophys., Texas A and M Univ., College  
Station, TX, 77843, USA  
SOURCE: Archives of Biochemistry and Biophysics (1980),  
204(1), 214-19  
CODEN: ABBIA4; ISSN: 0003-9861  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Kinetic measurements on the action of *Aeromonas* neutral protease toward  
blocked peptide substrates were made in order to det. the most favorable  
fit on the enzyme subsites that bind the residues flanking the scissile  
bond and to define the no. of secondary sites involved in catalysis.  
Variations in the identity of P1', the residue furnishing the amino group  
to the scissile bond, produced significant changes in kcat, whereas the  
identity of P1, the residue donating the carboxyl group, was of much less  
catalytic importance. Comparison of these results with those of previous  
investigators of the bacterial neutral proteases indicated distinct  
differences in specificity of the *Aeromonas* enzyme and revealed that  
phenylalanyl residues, rather than leucyl, were preferred in the P1'  
position. Addnl. binding sites on the carboxyl side of the scissile bond  
were shown to be important to catalytic efficiency, and it is evident that  
.gtoreq.3 residues (P1', P2', P3') are involved, whereas only 2 residues  
(P2, P1) on the N-terminal side of the sensitive bond are implicated.

IT **75501-77-8**

RL: BIOL (Biological study)  
(neutral protease of *Aeromonas* specificity for)

L5 ANSWER 31 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1980:501418 HCAPLUS  
DOCUMENT NUMBER: 93:101418  
TITLE: Degradation of side chains of N-(2-  
hydroxypropyl)methacrylamide copolymers by lysosomal  
enzymes  
AUTHOR(S): Duncan, Ruth; Lloyd, John B.; Kopecek, Jindrich  
CORPORATE SOURCE: Dep. Biol. Sci., Univ. Keele, Keele/Staffordshire, ST5  
5BG, UK  
SOURCE: Biochemical and Biophysical Research Communications  
(1980), 94(1), 284-90  
CODEN: BBRCA9; ISSN: 0006-291X

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A series of 22 N-(2-hydroxypropyl)methacrylamide copolymers, each contg. a  
different, potential degradable side chain, were incubated with rat liver  
tritosomes. Four of the side chains were digestible as judged by the  
liberation of a terminal 4-nitroaniline residue. The pH optimum for the  
degrdn. of the side chain -.epsilon.-aminocaproyl-phenylalanyl-4-  
nitroanilide was in the range 5.75-6.5 over the first hour of incubation  
and somewhat lower (pH 5.5-6.0) after this time. The degrdn. of the above  
side chain had a Km value of 58.3 mg/mL. The use of these compds. as drug  
carrier mols. is discussed.

IT **74569-71-4DP**, reaction products with N-

(hydroxypropyl)methacrylamide-methacrylamide copolymers  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and degrdn. of, by lysosomal enzymes, drug carrier in relation  
to)

L5 ANSWER 32 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1980:495630 HCAPLUS  
DOCUMENT NUMBER: 93:95630  
TITLE: N-Acylated phenylalanine p-nitroanilides: new  
substrates for chymotrypsin  
AUTHOR(S): Kasafirek, Evzen; Bartik, Michal  
CORPORATE SOURCE: Res. Inst. Pharm. Biochem., Prague, 130 60/3, Czech.  
SOURCE: Collection of Czechoslovak Chemical Communications

(1980), 45(2), 442-51  
CODEN: CCCCCK; ISSN: 0366-547X

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB R-Phe-NHC6H4NO2-p (R = Ac, HO2CCH:CHCO, MeOCH2CH2OCH2CO, HOCH2CO, H-Gly), H-Gly-Tyr-NHC6H4NO2-p, HO2CCH2CH2CO-X-Phe-NHC6H4NO2-4 (I; X = Gly, Gly-Gly, Gly-Gly-Gly), HO2CCH2CH2CO-X-Tyr-NHC6H4NO2-p (II; X = null, Gly, Gly-Gly), and Ac-His-Gly-Gly-Phe-NHC6H4NO2-p (III) were prepd. as substrates for chymotrypsin. Kinetic data for the cleavage of the above nitroanilides by chymotrypsin showed that the greatest kcat values were obtained for I (X = Gly-Gly) and II (X = Gly-Gly), and III produced the smallest Km value.

IT **74578-54-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and deblocking of)

IT **74569-71-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

IT **67877-92-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as substrate for chymotrypsin)

L5 ANSWER 33 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1978:575672 HCAPLUS

DOCUMENT NUMBER: 89:175672

TITLE: Modulation of the catalytic properties of  
.alpha.-chymotrypsin by chemical modification at Tyr  
146

AUTHOR(S): Gorecki, Marian; Wilchek, Meir; Blumberg, Shmaryahu

CORPORATE SOURCE: Dep. Chem., Weizmann Inst. Sci., Rehovot, Israel

SOURCE: Biochimica et Biophysica Acta (1978), 535(1), 90-9

CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE: Journal

LANGUAGE: English

AB .alpha.-Chymotrypsin was modified with 3 different diazonium salts derived from D-phenylalanine. All 3 reagents reacted selectively with tyrosine-146 on the surface of the enzyme. The spectral and enzymic properties of the azochymotrypsins were characteristic for each of the proteins. Depending on the structure of the reagent used for modification, the activity towards p-nitroanilide substrate was higher or about the same as that of the native enzyme.

IT **67877-92-3**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with azochymotrypsin, kinetics of)

L5 ANSWER 34 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:13107 HCAPLUS

DOCUMENT NUMBER: 86:13107

TITLE: Enzymic cleavage of side chains of synthetic  
water-soluble polymers

AUTHOR(S): Drobnik, J.; Kopecek, J.; Labsky, J.; Rejmanova, P.;

Exner, J.; Saudek, V.; Kalal, J.

CORPORATE SOURCE: Inst. Macromol. Chem., Czech. Acad. Sci., Prague,  
Czech.

SOURCE: Makromolekulare Chemie (1976), 177(10), 2833-48

CODEN: MACEAK; ISSN: 0025-116X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Water-sol. copolymers based on poly[N-(2-hydroxypropyl)methacrylamide] and bearing in their side chains a chromogenic substrate for chymotrypsin (EC 3.4.4.5) were prepd. by direct copolymerization or polymeranalogous reaction. The substrate was L-phenylalanine-4'-nitroanilide linked by its amino

group to the terminal carboxylic group of the side chain. The cleavage of the substrate thus bonded, was expressed by means of the Michaelis const., the max. velocity of the percentage of substrate unit accessible to the enzyme. The effect of length and chem. structure of the side chain was investigated in the first place. It was found that the chain must be longer than 6 atoms; longer chains are generally more favorable for this cleavage. The .epsilon.-aminocaproyl group provides a chain that is most favorable for the cleavage, whereas chains with several glycine units, though longer, are less favorable. Polymers with higher content of the substrate units undergo cleavage more readily.

IT **61435-98-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. and enzymic hydrolysis of)

IT **61435-72-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L5 ANSWER 35 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:101503 HCAPLUS

DOCUMENT NUMBER: 84:101503

TITLE: Bovine procarboxypeptidase A: kinetics of peptide and ester hydrolysis

AUTHOR(S): Bazzone, Thomas J.; Vallee, Bert L.

CORPORATE SOURCE: Dep. Biol. Chem., Harvard Med. Sch., Boston, MA, USA

SOURCE: Biochemistry (1976), 15(4), 868-75

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The kinetics of hydrolysis of a series of peptide and ester substrates by native procarboxypeptidase was examd. in detail in order to ascertain the extent to which the binding and catalytic sites of carboxypeptidase preexist in the zymogen. Distinct differences in the substrate binding sites of the zymogen compared to those of the enzyme are apparent from their resp. kinetic profiles as well as from the effects of modifiers on their activities. Substrate activation with the dipeptides BzGly-L-Phe and CbzGly-L-Phe, well known for carboxypeptidase, was exhibited also by the zymogen, but the corresponding substrate inhibition by CbzGly-L-Phe and BzGly-OPhe was absent. Moreover, the substrate inhibition of carboxypeptidase by CbzGlyGly-L-Phe and BzGly-OPhe was replaced by substrate activation in the zymogen. Benzoylglycine and cyclohexanol, potent modifiers of carboxypeptidase hydrolysis of peptides, barely affected the corresponding zymogen activities. Addnl., .beta.-phenylpropionate, a noncompetitive inhibitor of carboxypeptidase hydrolysis of peptides, competitively inhibited zymogen peptidase activity. Metal removal and substitution of Co for Zn in the zymogen resulted in effects on activity similar to those for carboxypeptidase, indicating that this component of the catalytic site is relatively unchanged in the process of zymogen activation. On the other hand, the pH dependence of peptidase activity and CO<sub>2</sub>H group modification both indicate an altered environment and reactivity for the catalytically essential CO<sub>2</sub>H group of Glu-270, consistent with the reduced catalytic efficiency of the zymogen. However, since the hydrolytic efficiency of the zymogen relative to the enzyme varies widely with substrate compn., the difference in CO<sub>2</sub>H group reactivity cannot account entirely for the obsd. differences in kinetic behavior of the zymogen and enzyme. Thus, while the essential features of the binding and catalytic sites of carboxypeptidase preexist in the zymogen, activation results in alterations in both of these active site components to generate the ultimate specificity and capacity of the enzyme.

IT **24848-63-3 58688-92-9**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of, kinetics of enzymic)

L5 ANSWER 36 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1972:498334 HCAPLUS  
DOCUMENT NUMBER: 77:98334  
TITLE: Distance measurements at the active site of  
carboxypeptidase A during catalysis  
AUTHOR(S): Latt, S. A.; Auld, D. S.; Vallee, B. L.  
CORPORATE SOURCE: Dep. Biol. Chem., Harvard Med. Sch., Boston, MA, USA  
SOURCE: Biochemistry (1972), 11(16), 3015-22  
CODEN: BICHAW; ISSN: 0006-2960  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Both native Zn carboxypeptidase A and the Co-substituted deriv. rapidly hydrolyze 2 new series of peptides, dansyl-(Gly)n-L-Phe(n = 1, 2, 3, 4) and dansyl-(Gly)n-L-Trp (n = 1, 2, 3). In conjunction with Co carboxypeptidase these substrates simultaneously afford measurements of kinetic parameters and of distances within and topographical features of the enzyme active center. For Zn carboxypeptidase, values of kcat range from 4 .times. 10<sup>1</sup> to 1 .times. 10<sup>4</sup> min<sup>-1</sup> and values of Km from 8 .times. 10<sup>-5</sup> to 1 .times. 10<sup>-3</sup>M. For the Co enzyme, the corresponding kcat values are 1.5-4 times higher and the Km values are .apprx.0.5 lower. Distance measurements are based on electronic energy transfer. The dansyl group serves both as an acceptor of tryptophanyl excitation energy and as its donor to the Co atom in a tryptophan-dansyl-Co energy-relay system. Energy transfer between enzyme tryptophanyl residues and substrate dansyl groups rapidly identifies the formation and breakdown of enzyme-substrate complexes. Subsequent transfer of energy from the bound dansyl group to the Co atom allows calcn. of the distance between these moieties when dipole-dipole resonance computed in this manner increase systematically from <8 .ANG. for the dipeptides to .apprx.15 .ANG. for the pentapeptides. The values for corresponding members of the phenylalanyl and tryptophanyl series of substrates are in good agreement with each other. They also compare favorably to distances estd. from mol. models assuming an extended peptide to interact with the Co atom at the carbonyl O of the bond to be split. The measurement of catalysis related distances in other enzyme active centers should be possible through the incorporation of suitable spectrochem. probes into both the substrate and the enzyme.

IT 37923-00-5

RL: BIOL (Biological study)  
(reaction with carboxypeptidase A, kinetics of)

L5 ANSWER 37 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1971:498805 HCAPLUS  
DOCUMENT NUMBER: 75:98805  
TITLE: Peptides with terminal tyrosyl and phenylalanyl groups  
AUTHOR(S): Skorc, Joseph A.  
CORPORATE SOURCE: Lakeside Lab., Colgate-Palmolive Co., Milwaukee, WI, USA  
SOURCE: Journal of Medicinal Chemistry (1971), 14(8), 775-6  
CODEN: JCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Three tripeptides and a pentapeptide contg. both N-terminal L-tyrosyl and C-terminal L-phenylalanyl groups, were prepd. for general cardiovascular evaluation in dogs. Only 1-L-tyrosylamino-1-cyclopentyl-L-phenylalanine acetate at 1 mg/ kg, i.v., caused a marked, transient decrease in blood pressure, but did not inhibit angiotensin-induced contractions of the isolated rat uterus at concns. up to 10 .mu.g/ml.

IT 33374-78-6P 33492-41-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L5 ANSWER 38 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN



ACCESSION NUMBER: 1970:474039 HCAPLUS  
DOCUMENT NUMBER: 73:74039  
TITLE: Bacterial utilization of oligopeptides containing  
.beta.-2-thienylalanine and phenylalanine  
AUTHOR(S): Smith, Robert Lewis; Dunn, Floyd W.  
CORPORATE SOURCE: Coll. of Basic Bed. Sci., Univ. of Tennessee, Memphis,  
TN, USA  
SOURCE: Journal of Biological Chemistry (1970), 245(11),  
2962-6  
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A series of tetrapeptides including triglycyl-DL-phenylalanine, DL-phenylalanyltriglycine, triglycyl-.beta.-2-thienyl-DL-alanine, and .beta.-2-thienyl-DL-alanyltriglycine was synthesized by conventional methods. The 2 pentapeptides L-phenylalanyltetraglycine and .beta.-2-thienyl-L-alanyltetraglycine were synthesized by a solid phase method. The peptides were tested for their capacity to influence the growth of a wild strain of Escherichia coli. The 2 tetrapeptides contg. .beta.-2-thienylalanine were good inhibitors of E. coli growth in basal medium; however, the pentapeptide was inhibitory only at relatively high concns. The 2 tetrapeptides contg. phenylalanine were more efficient in reversing the growth inhibitory effects of .beta.-2-thienylalanine than was free phenylalanine, but the pentapeptide L-phenylalanyltetraglycine stimulated E. coli growth only at high concns. in the presence of .beta.-2-thienylalanine. When E. coli growth was dependent upon the presence of either DL-phenylalanyltriglycine or triglycyl-DL-phenylalanine, the analogous .beta.-2-thienylalanine in inhibiting E. coli growth. The results show that the growth of a wild strain of E. coli is influenced by several tetrapeptides contg. either phenylalanine or .beta.-2-thienylalanine. However, 2 pentapeptides were relatively ineffective, probably because of severely limited transport of these larger mols. into the cells.

IT 25894-99-9

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(metabolism of, by Escherichia coli)

L5 ANSWER 39 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1970:18693 HCAPLUS  
DOCUMENT NUMBER: 72:18693  
TITLE: Pyridyl esters of peptides as synthetic substrates of pepsin  
AUTHOR(S): Sachdev, Goverdhan P.; Fruton, Joseph S.  
CORPORATE SOURCE: Yale Univ., New Haven, CT, USA  
SOURCE: Biochemistry (1969), 8(11), 4231-8  
CODEN: BICHAW; ISSN: 0006-2960  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The synthesis of a series of new pepsin substrates of the type A-Phe-Phe-B is described, in which B is a pyridylalkyloxy group, A is benzyloxycarbonyl (Z), Z-Gly, or Z-Gly-Gly, and the Phe-Phe linkage is the only pepsin-sensitive bond. In their cationic form, these compds. are moderately sol. in aq. soln. at pH 2-4, and some of the compds. (e.g., with A = Z-Gly-Gly) are among the most sensitive synthetic substrates hitherto found for pepsin. The detn. of the kinetic parameters for their enzymic hydrolysis has shown that changes in the structure of the A and B groups of A-Phe-Phe-B may have very large effects on the value of kcat (.apprx.500-fold change) with only small accompanying changes in the value of KM. These kinetic data emphasize the importance, for the kinetic specificity of pepsin, of interactions between the A or B groups of the substrate with enzymic loci that are relatively distant from the site of catalytic action, and are consistent with the possibility that such

secondary interactions may alter the conformation of catalytically important groups in the enzyme so as to alter greatly the efficiency of catalysis.

IT 26108-22-5

RL: BIOL (Biological study)  
(as pepsin substrate)

L5 ANSWER 40 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1965:52017 HCAPLUS  
DOCUMENT NUMBER: 62:52017  
ORIGINAL REFERENCE NO.: 62:9233h,9234a  
TITLE: Synthesis of polypeptides with known repeating sequence of amino acids  
AUTHOR(S): Kovacs, J.; Kapoor, A.  
CORPORATE SOURCE: St. John's Univ., New York, NY  
SOURCE: Journal of the American Chemical Society (1965), 87(1), 118-19  
CODEN: JACSAT; ISSN: 0002-7863  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB cf. Pless and Boissonas, *Helv. Chim. Acta* 46, 1609-25(1963). Polypeptides with known repeating sequence of amino acids were prepd. from pentachlorophenyl active esters. Thus were prepd. poly(.alpha.-L-glutamyl-L-alanyl-L-glutamic acid) (mol. wt. 20,000), poly(glycylglycyl-L-phenylalanine), and poly(.gamma.-L-glutamyl-.gamma.-aminobutyric acid).

IT 3017-43-4, 1,4,7,10-Tetraazacyclododecane-2,5,8,11-tetrone, 3-benzyl-  
(prepn. of)

L5 ANSWER 41 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1965:52016 HCAPLUS  
DOCUMENT NUMBER: 62:52016  
ORIGINAL REFERENCE NO.: 62:9233g-h  
TITLE: Cyclization of glycyl-phenylalanine tetrapeptides  
AUTHOR(S): Morozova, E. A.; Ionova, L. V.; Drobinskaya, N. A.  
CORPORATE SOURCE: M. V. Lomonosov State Univ., Moscow  
SOURCE: *Zhurnal Obshchei Khimii* (1964), 34(12), 3888-90  
CODEN: ZOKHA4; ISSN: 0044-460X  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian

AB Heating the tetrapeptides (Phe-Gly-Gly-Gly, decompd. 198-201.degree.; Gly-Phe-Gly-Gly, decompd. 185-6.degree.; Gly-Gly-Phe-Gly, decompd. 204-5.degree.; Gly-Gly-Gly-Phe, decompd. 195-7.degree.) in MeOH with 10-fold excess EtOC:CH 12 hrs. at 70.degree. and keeping the mixt. overnight at room temp. gave after evapn. and electrophoretic sepn. on cellulose powder in 30% AcOH, the following cyclotetrapeptides: cyclo-(Phe-Gly-Gly-Gly), decompd. 250-300.degree.; cyclo-(Gly-Phe-Gly-Gly), decompd. 250-300.degree.; cyclo-(Gly-Gly-Phe-Gly), decompd. 250-300.degree.; cyclo-(Gly-Gly-Gly-Phe), decompd. 250-300.degree.; the yields were 17%, 9.25%, 10.6%, and 23.4%, resp. The products were characterized by partial hydrolysis in hot aq. LiOH 15 min. The mol. wts. of the cyclopeptides were checked by isothermal distn. with HCO<sub>2</sub>H.

IT 3017-43-4, 1,4,7,10-Tetraazacyclododecane-2,5,8,11-tetrone, 3-benzyl-  
(prepn. of)

L5 ANSWER 42 OF 42 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1964:469405 HCAPLUS  
DOCUMENT NUMBER: 61:69405  
ORIGINAL REFERENCE NO.: 61:12079d-g  
TITLE: Synthesis of glycyl-leucine and glycyl-phenylalanine tetrapeptides  
AUTHOR(S): Ionova, L. V.; Morozova, E. A.; Pliner, S. A.;

SOURCE: Drobinskaya, N. A.  
Vestnik Moskovskogo Universiteta, Seriya 2: Khimiya  
(1964), 19(4), 85-9  
CODEN: VMUKA5; ISSN: 0579-9384  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

- AB A series of Me esters of acyl peptides was prepd. by reaction of the Me ester of an amino acid or peptide with a carbobenzoxyated (Z = PhCH<sub>2</sub>O<sub>2</sub>C) amino acid or peptide. The peptide bond was formed by the mixed anhydride method. Sapon. of the acyl peptide ester led to the corresponding carbobenzoxyated peptide acid. Redn. of the Z group with H and Pd catalyst in the presence of 1 equiv. HOAc gave the free peptide. Thus prepd. were Z-Gly-Gly-Leu(OMe), m. 124.degree.; Z-Gly-Gly-Leu(OH), m. 175-6.degree.; Z-Gly-Gly-Phe(OMe).0.5H<sub>2</sub>O, m. 96-7.degree.; Z-Gly-Gly-Phe(OH), m. 143-4.degree.; Z-Gly-Gly-Gly-Leu(OMe), m. 150-5.degree.; Z-Gly-Gly-Gly-Leu(OH), m. 176-8.degree.; H-Gly-Gly-Gly-Leu(OH), m. 206-7.degree.; Z-Gly-Gly-Leu-Gly(OMe), m. 123-6.degree.; Z-Gly-Gly-Leu-Gly(OH), m. 150-2.degree.; H-Gly-Gly-Leu-Gly(OH).3H<sub>2</sub>O, m. 172-5.degree.; Z-Gly-Leu-Gly-Gly(OMe), m. 89-94.degree.; Z-Gly-Leu-Gly-Gly(OH), m. 178-80.degree.; H-Gly-Leu-Gly-Gly(OH).0.5H<sub>2</sub>O, m. 166-70.degree.; Z-Gly-Gly-Gly-Phe(OMe), m. 114-16.degree.; Z-Gly-Gly-Gly-Phe(OH), m. 167-8.degree.; H-Gly-Gly-Gly-Phe(OH).0.5H<sub>2</sub>O, m. 195-7.degree.; Z-Gly-Gly-Phe-Gly(OMe), m. 101.degree.; Z-Gly-Gly-Phe-Gly(OH), m. 120.degree.; H-Gly-Gly-Phe-Gly(OH).1.5H<sub>2</sub>O, m. 204-5.degree.; Z-Gly-Phe-Gly-Gly(OMe), m. 124-6.degree.; Z-Gly-Phe-Gly-Gly(OH), m. 152-4.degree.; H-Gly-Phe-Gly-Gly.1.5H<sub>2</sub>O, m. 185-6.degree.; Z-Phe-Gly-Gly-Gly(OMe).1.5H<sub>2</sub>O, m. 171-2.degree.; Z-Phe-Gly-Gly-Gly(OH), m. 137-9.degree.; H-Phe-Gly-Gly-Gly(OH).1.5H<sub>2</sub>O, m. 198-201.degree.. The R<sub>f</sub> values for the free peptides were given.
- IT **24848-63-3**, Alanine, N-[N-[N-(N-carboxyglycyl)glycyl]glycyl]-3-phenyl-, N-benzyl ester **33374-78-6**, Alanine, N-[N-[N-(N-carboxyglycyl)glycyl]glycyl]-3-phenyl-, N-benzyl Me ester **75853-32-6**, Alanine, N-[N-(N-glycylglycyl)glycyl]-3-phenyl- (prepn. of)

=>

=> fil reg

FILE 'REGISTRY' ENTERED AT 14:24:54 ON 21 OCT 2003  
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STRUCTURE FILE UPDATES: 20 OCT 2003 HIGHEST RN 607332-91-2  
DICTIONARY FILE UPDATES: 20 OCT 2003 HIGHEST RN 607332-91-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

```
=> d .seq 14 tot
```

| type         | location | description                        |
|--------------|----------|------------------------------------|
| modification | Gly-1    | (1,1-dimethylethoxy) carbonyl<Boc> |
| modification | Phe-4    | undetermined modification          |

```

SEQ      1  GGGF
          ==
HITS AT:  1-4

```

\*\*RELATED SEQUENCES AVAILABLE WITH SEOLINK\*\*

REFERENCE 1: 136:402018

| type         | location | description                        |
|--------------|----------|------------------------------------|
| modification | Gly-1    | (1,1-dimethylethoxy) carbonyl<Boc> |
| modification | Phe-4    | undetermined modification          |

```

SEQ      1  GGGF
          ==
HITS AT: 1-4

```

\*\*RELATED SEOUENCES AVAILABLE WITH SEOLINK\*\*

REFERENCE 1: 136:402018

```

.type          ----- location -----      description

```

|          |            |              |                 |
|----------|------------|--------------|-----------------|
| bridge   | Orn-6      | - Gly-4[12'] | amide bridge    |
| bridge   | Orn-10     | - Gly-8[6']  | amide bridge    |
| bridge   | Orn-14     | - Gly-12'''  | amide bridge    |
| bridge   | Phe-18     | - Phe-18'    | covalent bridge |
| bridge   | Phe-18     | - Phe-18''   | covalent bridge |
| bridge   | Orn-6'     | - Gly-4[16'] | amide bridge    |
| bridge   | Orn-10'    | - Gly-8[8']  | amide bridge    |
| bridge   | Orn-14'    | - Gly-12[4'] | amide bridge    |
| bridge   | Phe-18'    | - Phe-18''   | covalent bridge |
| bridge   | Orn-6''    | - Gly-4[20'] | amide bridge    |
| bridge   | Orn-10''   | - Gly-8[10'] | amide bridge    |
| bridge   | Orn-14''   | - Gly-12[5'] | amide bridge    |
| bridge   | Orn-6'''   | - Gly-4[14'] | amide bridge    |
| bridge   | Orn-10'''  | - Gly-8[7']  | amide bridge    |
| bridge   | Orn-6[4']  | - Gly-4[18'] | amide bridge    |
| bridge   | Orn-10[4'] | - Gly-8[9']  | amide bridge    |
| bridge   | Orn-6[5']  | - Gly-4[22'] | amide bridge    |
| bridge   | Orn-10[5'] | - Gly-8[11'] | amide bridge    |
| bridge   | Orn-6[6']  | - Gly-4[13'] | amide bridge    |
| bridge   | Orn-6[7']  | - Gly-4[15'] | amide bridge    |
| bridge   | Orn-6[8']  | - Gly-4[17'] | amide bridge    |
| bridge   | Orn-6[9']  | - Gly-4[19'] | amide bridge    |
| bridge   | Orn-6[10'] | - Gly-4[21'] | amide bridge    |
| bridge   | Orn-6[11'] | - Gly-4[23'] | amide bridge    |
| uncommon | Orn-2      | -            | -               |
| uncommon | Orn-6      | -            | -               |
| uncommon | Orn-10     | -            | -               |
| uncommon | Orn-14     | -            | -               |
| uncommon | Orn-2'     | -            | -               |
| uncommon | Orn-6'     | -            | -               |
| uncommon | Orn-10'    | -            | -               |
| uncommon | Orn-14'    | -            | -               |
| uncommon | Orn-2''    | -            | -               |
| uncommon | Orn-6''    | -            | -               |
| uncommon | Orn-10''   | -            | -               |
| uncommon | Orn-14''   | -            | -               |
| uncommon | Orn-2'''   | -            | -               |
| uncommon | Orn-6'''   | -            | -               |
| uncommon | Orn-10'''  | -            | -               |
| uncommon | Orn-2[4']  | -            | -               |
| uncommon | Orn-6[4']  | -            | -               |
| uncommon | Orn-10[4'] | -            | -               |
| uncommon | Orn-2[5']  | -            | -               |
| uncommon | Orn-6[5']  | -            | -               |
| uncommon | Orn-10[5'] | -            | -               |
| uncommon | Orn-2[6']  | -            | -               |
| uncommon | Orn-6[6']  | -            | -               |
| uncommon | Orn-2[7']  | -            | -               |
| uncommon | Orn-6[7']  | -            | -               |
| uncommon | Orn-2[8']  | -            | -               |
| uncommon | Orn-6[8']  | -            | -               |
| uncommon | Orn-2[9']  | -            | -               |
| uncommon | Orn-6[9']  | -            | -               |
| uncommon | Orn-2[10'] | -            | -               |
| uncommon | Orn-6[10'] | -            | -               |
| uncommon | Orn-2[11'] | -            | -               |
| uncommon | Orn-6[11'] | -            | -               |
| uncommon | Orn-2[12'] | -            | -               |
| uncommon | Orn-2[13'] | -            | -               |
| uncommon | Orn-2[14'] | -            | -               |
| uncommon | Orn-2[15'] | -            | -               |
| uncommon | Orn-2[16'] | -            | -               |

|          |            |   |   |
|----------|------------|---|---|
| uncommon | Orn-2[17'] | - | - |
| uncommon | Orn-2[18'] | - | - |
| uncommon | Orn-2[19'] | - | - |
| uncommon | Orn-2[20'] | - | - |
| uncommon | Orn-2[21'] | - | - |
| uncommon | Orn-2[22'] | - | - |
| uncommon | Orn-2[23'] | - | - |

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

```

SEQ      1  GXGGGXGGGX  GGGXGGGF
                               =====

```

**\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\***

L4 ANSWER 4 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

CN L-Phenylalaninamide, 18,18''''''''',18''''''''''''''''''-(nitrilotri-2,1-ethanediyl) tris[N-acetylglucyl-N5-acetyl-L-ornithylglycylglycylglycyl-N5-(N-acetylglucyl-N5-acetyl-L-ornithylglycylglycyl)-L-ornithylglycylglycylglycyl-N5-[N-acetylglucyl-N5-acetyl-L-ornithylglycylglycylglycyl-N5-(N-acetylglucyl-N5-acetyl-L-ornithylglycylglycyl)-L-ornithylglycylglycyl]-L-ornithylglycylglycylglycyl-N5-[N-acetylglucyl-N5-acetyl-L-ornithylglycylglycylglycyl-N5-(N-acetylglucyl-N5-acetyl-L-ornithylglycylglycyl)-L-ornithylglycylglycylglycyl-N5-[N-acetylglucyl-N5-acetyl-L-

ornithylglycylglycylglycyl-N5-(N-acetylglycyl-N5-acetyl-L-  
 ornithylglycylglycyl)-L-ornithylglycylglycyl]-L-ornithylglycylglycyl]-L-  
 ornithylglycylglycyl- (9CI) (CA INDEX NAME)

NTE multichain

modified (modifications unspecified)

| type     | -----      | location | -----      | description     |
|----------|------------|----------|------------|-----------------|
| bridge   | Orn-6      | -        | Gly-4[12'] | amide bridge    |
| bridge   | Orn-10     | -        | Gly-8[6']  | amide bridge    |
| bridge   | Orn-14     | -        | Gly-12'''  | amide bridge    |
| bridge   | Phe-18     | -        | Phe-18'    | covalent bridge |
| bridge   | Phe-18     | -        | Phe-18''   | covalent bridge |
| bridge   | Orn-6'     | -        | Gly-4[16'] | amide bridge    |
| bridge   | Orn-10'    | -        | Gly-8[8']  | amide bridge    |
| bridge   | Orn-14'    | -        | Gly-12[4'] | amide bridge    |
| bridge   | Phe-18'    | -        | Phe-18''   | covalent bridge |
| bridge   | Orn-6''    | -        | Gly-4[20'] | amide bridge    |
| bridge   | Orn-10''   | -        | Gly-8[10'] | amide bridge    |
| bridge   | Orn-14''   | -        | Gly-12[5'] | amide bridge    |
| bridge   | Orn-6'''   | -        | Gly-4[14'] | amide bridge    |
| bridge   | Orn-10'''  | -        | Gly-8[7']  | amide bridge    |
| bridge   | Orn-6[4']  | -        | Gly-4[18'] | amide bridge    |
| bridge   | Orn-10[4'] | -        | Gly-8[9']  | amide bridge    |
| bridge   | Orn-6[5']  | -        | Gly-4[22'] | amide bridge    |
| bridge   | Orn-10[5'] | -        | Gly-8[11'] | amide bridge    |
| bridge   | Orn-6[6']  | -        | Gly-4[13'] | amide bridge    |
| bridge   | Orn-6[7']  | -        | Gly-4[15'] | amide bridge    |
| bridge   | Orn-6[8']  | -        | Gly-4[17'] | amide bridge    |
| bridge   | Orn-6[9']  | -        | Gly-4[19'] | amide bridge    |
| bridge   | Orn-6[10'] | -        | Gly-4[21'] | amide bridge    |
| bridge   | Orn-6[11'] | -        | Gly-4[23'] | amide bridge    |
| uncommon | Orn-2      | -        | -          | -               |
| uncommon | Orn-6      | -        | -          | -               |
| uncommon | Orn-10     | -        | -          | -               |
| uncommon | Orn-14     | -        | -          | -               |
| uncommon | Orn-2'     | -        | -          | -               |
| uncommon | Orn-6'     | -        | -          | -               |
| uncommon | Orn-10'    | -        | -          | -               |
| uncommon | Orn-14'    | -        | -          | -               |
| uncommon | Orn-2''    | -        | -          | -               |
| uncommon | Orn-6''    | -        | -          | -               |
| uncommon | Orn-10''   | -        | -          | -               |
| uncommon | Orn-14''   | -        | -          | -               |
| uncommon | Orn-2'''   | -        | -          | -               |
| uncommon | Orn-6'''   | -        | -          | -               |
| uncommon | Orn-10'''  | -        | -          | -               |
| uncommon | Orn-2[4']  | -        | -          | -               |
| uncommon | Orn-6[4']  | -        | -          | -               |
| uncommon | Orn-10[4'] | -        | -          | -               |
| uncommon | Orn-2[5']  | -        | -          | -               |
| uncommon | Orn-6[5']  | -        | -          | -               |
| uncommon | Orn-10[5'] | -        | -          | -               |
| uncommon | Orn-2[6']  | -        | -          | -               |
| uncommon | Orn-6[6']  | -        | -          | -               |
| uncommon | Orn-2[7']  | -        | -          | -               |
| uncommon | Orn-6[7']  | -        | -          | -               |
| uncommon | Orn-2[8']  | -        | -          | -               |
| uncommon | Orn-6[8']  | -        | -          | -               |
| uncommon | Orn-2[9']  | -        | -          | -               |
| uncommon | Orn-6[9']  | -        | -          | -               |
| uncommon | Orn-2[10'] | -        | -          | -               |
| uncommon | Orn-6[10'] | -        | -          | -               |

|          |            |   |   |
|----------|------------|---|---|
| uncommon | Orn-2[11'] | - | - |
| uncommon | Orn-6[11'] | - | - |
| uncommon | Orn-2[12'] | - | - |
| uncommon | Orn-2[13'] | - | - |
| uncommon | Orn-2[14'] | - | - |
| uncommon | Orn-2[15'] | - | - |
| uncommon | Orn-2[16'] | - | - |
| uncommon | Orn-2[17'] | - | - |
| uncommon | Orn-2[18'] | - | - |
| uncommon | Orn-2[19'] | - | - |
| uncommon | Orn-2[20'] | - | - |
| uncommon | Orn-2[21'] | - | - |
| uncommon | Orn-2[22'] | - | - |
| uncommon | Orn-2[23'] | - | - |

SQL 186,18,18,18,12,12,12,8,8,8,8,8,8,4,4,4,  
4,4,4,4,4,4,  
4,4,4

SQL 186,18,18,18,12,12,12,8,8,8,8,8,8,4,4,4,  
4,4,4,4,4,4,  
4,4,4

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 134:147856

L4 ANSWER 5 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 323178-50-3 REGISTRY

CN L-Phenylalaninamide, 18,18''''''''',18''''''''''''''''''''-(nitrilotri-2,1-ethanediyl)tris[glycyl-L-ornithylglycylglycylglycyl-N5-(glycyl-L-



ornithylglycylglycyl)-L-ornithylglycylglycylglycyl-N5-[glycyl-L-  
 ornithylglycylglycylglycyl-N5-(glycyl-L-ornithylglycylglycyl)-L-  
 ornithylglycylglycyl)-L-ornithylglycylglycylglycyl-N5-[glycyl-L-  
 ornithylglycylglycylglycyl-N5-(glycyl-L-ornithylglycylglycyl)-L-  
 ornithylglycylglycylglycyl-N5-[glycyl-L-ornithylglycylglycylglycyl-N5-  
 (glycyl-L-ornithylglycylglycyl)-L-ornithylglycylglycyl)-L-  
 ornithylglycylglycyl)-L-ornithylglycylglycyl-, trifluoroacetate (9CI) (CA  
 INDEX NAME)

NTE multichain  
 modified (modifications unspecified)

| type     | location   |              | description     |
|----------|------------|--------------|-----------------|
| bridge   | Orn-6      | - Gly-4[12'] | amide bridge    |
| bridge   | Orn-10     | - Gly-8[6']  | amide bridge    |
| bridge   | Orn-14     | - Gly-12'''  | amide bridge    |
| bridge   | Phe-18     | - Phe-18'    | covalent bridge |
| bridge   | Phe-18     | - Phe-18''   | covalent bridge |
| bridge   | Orn-6'     | - Gly-4[16'] | amide bridge    |
| bridge   | Orn-10'    | - Gly-8[8']  | amide bridge    |
| bridge   | Orn-14'    | - Gly-12[4'] | amide bridge    |
| bridge   | Phe-18'    | - Phe-18''   | covalent bridge |
| bridge   | Orn-6''    | - Gly-4[20'] | amide bridge    |
| bridge   | Orn-10''   | - Gly-8[10'] | amide bridge    |
| bridge   | Orn-14''   | - Gly-12[5'] | amide bridge    |
| bridge   | Orn-6'''   | - Gly-4[14'] | amide bridge    |
| bridge   | Orn-10'''  | - Gly-8[7']  | amide bridge    |
| bridge   | Orn-6[4']  | - Gly-4[18'] | amide bridge    |
| bridge   | Orn-10[4'] | - Gly-8[9']  | amide bridge    |
| bridge   | Orn-6[5']  | - Gly-4[22'] | amide bridge    |
| bridge   | Orn-10[5'] | - Gly-8[11'] | amide bridge    |
| bridge   | Orn-6[6']  | - Gly-4[13'] | amide bridge    |
| bridge   | Orn-6[7']  | - Gly-4[15'] | amide bridge    |
| bridge   | Orn-6[8']  | - Gly-4[17'] | amide bridge    |
| bridge   | Orn-6[9']  | - Gly-4[19'] | amide bridge    |
| bridge   | Orn-6[10'] | - Gly-4[21'] | amide bridge    |
| bridge   | Orn-6[11'] | - Gly-4[23'] | amide bridge    |
| uncommon | Orn-2      | -            | -               |
| uncommon | Orn-6      | -            | -               |
| uncommon | Orn-10     | -            | -               |
| uncommon | Orn-14     | -            | -               |
| uncommon | Orn-2'     | -            | -               |
| uncommon | Orn-6'     | -            | -               |
| uncommon | Orn-10'    | -            | -               |
| uncommon | Orn-14'    | -            | -               |
| uncommon | Orn-2''    | -            | -               |
| uncommon | Orn-6''    | -            | -               |
| uncommon | Orn-10''   | -            | -               |
| uncommon | Orn-14''   | -            | -               |
| uncommon | Orn-2'''   | -            | -               |
| uncommon | Orn-6'''   | -            | -               |
| uncommon | Orn-10'''  | -            | -               |
| uncommon | Orn-2[4']  | -            | -               |
| uncommon | Orn-6[4']  | -            | -               |
| uncommon | Orn-10[4'] | -            | -               |
| uncommon | Orn-2[5']  | -            | -               |
| uncommon | Orn-6[5']  | -            | -               |
| uncommon | Orn-10[5'] | -            | -               |
| uncommon | Orn-2[6']  | -            | -               |
| uncommon | Orn-6[6']  | -            | -               |
| uncommon | Orn-2[7']  | -            | -               |
| uncommon | Orn-6[7']  | -            | -               |
| uncommon | Orn-2[8']  | -            | -               |

|          |            |   |   |
|----------|------------|---|---|
| uncommon | Orn-6[8']  | - | - |
| uncommon | Orn-2[9']  | - | - |
| uncommon | Orn-6[9']  | - | - |
| uncommon | Orn-2[10'] | - | - |
| uncommon | Orn-6[10'] | - | - |
| uncommon | Orn-2[11'] | - | - |
| uncommon | Orn-6[11'] | - | - |
| uncommon | Orn-2[12'] | - | - |
| uncommon | Orn-2[13'] | - | - |
| uncommon | Orn-2[14'] | - | - |
| uncommon | Orn-2[15'] | - | - |
| uncommon | Orn-2[16'] | - | - |
| uncommon | Orn-2[17'] | - | - |
| uncommon | Orn-2[18'] | - | - |
| uncommon | Orn-2[19'] | - | - |
| uncommon | Orn-2[20'] | - | - |
| uncommon | Orn-2[21'] | - | - |
| uncommon | Orn-2[22'] | - | - |
| uncommon | Orn-2[23'] | - | - |

---

SQL 186,18,18,18,12,12,12,8,8,8,8,8,8,4,4,4,  
4,4,4,4,4,4,  
4,4,4

SQL 186,18,18,18,12,12,12,8,8,8,8,8,8,4,4,4,  
4,4,4,4,4,4,  
4,4,4

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 134:147856

RN 323178-48-9 REGISTRY

CN L-Phenylalaninamide, 18,18''''''''',18''''''''''''''''''''-(nitrilotri-2,1-ethanediyl) tris[N-acetylglycyl-N5-acetyl-L-ornithylglycylglycylglycyl-N5-(N-acetylglycyl-N5-acetyl-L-ornithylglycylglycyl)-L-ornithylglycylglycylglycyl-N5-[N-acetylglycyl-N5-acetyl-L-ornithylglycylglycylglycyl-N5-(N-acetylglycyl-N5-acetyl-L-ornithylglycylglycyl)-L-ornithylglycylglycyl]-L-ornithylglycylglycylglycyl-N5-[N-acetylglycyl-N5-acetyl-L-ornithylglycylglycylglycyl-N5-(N-acetylglycyl-N5-acetyl-L-ornithylglycylglycyl)-L-ornithylglycylglycyl]-L-ornithylglycylglycylglycyl-N5-(N-acetylglycyl-N5-acetyl-L-ornithylglycylglycyl)-L-ornithylglycylglycylglycyl]-L-ornithylglycylglycylglycyl- (9CI) (CA INDEX NAME)

NTE multichain

modified (modifications unspecified)

| type     | -----      | location | -----      | description     |
|----------|------------|----------|------------|-----------------|
| bridge   | Orn-6      | -        | Gly-4[12'] | amide bridge    |
| bridge   | Orn-10     | -        | Gly-8[6']  | amide bridge    |
| bridge   | Orn-14     | -        | Gly-12'''  | amide bridge    |
| bridge   | Phe-18     | -        | Phe-18'    | covalent bridge |
| bridge   | Phe-18     | -        | Phe-18''   | covalent bridge |
| bridge   | Orn-6'     | -        | Gly-4[16'] | amide bridge    |
| bridge   | Orn-10'    | -        | Gly-8[8']  | amide bridge    |
| bridge   | Orn-14'    | -        | Gly-12[4'] | amide bridge    |
| bridge   | Phe-18'    | -        | Phe-18''   | covalent bridge |
| bridge   | Orn-6''    | -        | Gly-4[20'] | amide bridge    |
| bridge   | Orn-10''   | -        | Gly-8[10'] | amide bridge    |
| bridge   | Orn-14''   | -        | Gly-12[5'] | amide bridge    |
| bridge   | Orn-6'''   | -        | Gly-4[14'] | amide bridge    |
| bridge   | Orn-10'''  | -        | Gly-8[7']  | amide bridge    |
| bridge   | Orn-6[4']  | -        | Gly-4[18'] | amide bridge    |
| bridge   | Orn-10[4'] | -        | Gly-8[9']  | amide bridge    |
| bridge   | Orn-6[5']  | -        | Gly-4[22'] | amide bridge    |
| bridge   | Orn-10[5'] | -        | Gly-8[11'] | amide bridge    |
| bridge   | Orn-6[6']  | -        | Gly-4[13'] | amide bridge    |
| bridge   | Orn-6[7']  | -        | Gly-4[15'] | amide bridge    |
| bridge   | Orn-6[8']  | -        | Gly-4[17'] | amide bridge    |
| bridge   | Orn-6[9']  | -        | Gly-4[19'] | amide bridge    |
| bridge   | Orn-6[10'] | -        | Gly-4[21'] | amide bridge    |
| bridge   | Orn-6[11'] | -        | Gly-4[23'] | amide bridge    |
| uncommon | Orn-2      | -        | -          | -               |
| uncommon | Orn-6      | -        | -          | -               |
| uncommon | Orn-10     | -        | -          | -               |
| uncommon | Orn-14     | -        | -          | -               |
| uncommon | Orn-2'     | -        | -          | -               |
| uncommon | Orn-6'     | -        | -          | -               |
| uncommon | Orn-10'    | -        | -          | -               |
| uncommon | Orn-14'    | -        | -          | -               |
| uncommon | Orn-2''    | -        | -          | -               |
| uncommon | Orn-6''    | -        | -          | -               |
| uncommon | Orn-10''   | -        | -          | -               |
| uncommon | Orn-14''   | -        | -          | -               |
| uncommon | Orn-2'''   | -        | -          | -               |
| uncommon | Orn-6'''   | -        | -          | -               |
| uncommon | Orn-10'''  | -        | -          | -               |
| uncommon | Orn-2[4']  | -        | -          | -               |
| uncommon | Orn-6[4']  | -        | -          | -               |
| uncommon | Orn-10[4'] | -        | -          | -               |
| uncommon | Orn-2[5']  | -        | -          | -               |

|          |            |   |   |
|----------|------------|---|---|
| uncommon | Orn-6[5']  | - | - |
| uncommon | Orn-10[5'] | - | - |
| uncommon | Orn-2[6']  | - | - |
| uncommon | Orn-6[6']  | - | - |
| uncommon | Orn-2[7']  | - | - |
| uncommon | Orn-6[7']  | - | - |
| uncommon | Orn-2[8']  | - | - |
| uncommon | Orn-6[8']  | - | - |
| uncommon | Orn-2[9']  | - | - |
| uncommon | Orn-6[9']  | - | - |
| uncommon | Orn-2[10'] | - | - |
| uncommon | Orn-6[10'] | - | - |
| uncommon | Orn-2[11'] | - | - |
| uncommon | Orn-6[11'] | - | - |
| uncommon | Orn-2[12'] | - | - |
| uncommon | Orn-2[13'] | - | - |
| uncommon | Orn-2[14'] | - | - |
| uncommon | Orn-2[15'] | - | - |
| uncommon | Orn-2[16'] | - | - |
| uncommon | Orn-2[17'] | - | - |
| uncommon | Orn-2[18'] | - | - |
| uncommon | Orn-2[19'] | - | - |
| uncommon | Orn-2[20'] | - | - |
| uncommon | Orn-2[21'] | - | - |
| uncommon | Orn-2[22'] | - | - |
| uncommon | Orn-2[23'] | - | - |

---

SQL 186,18,18,18,12,12,12,8,8,8,8,8,8,4,4,4,  
4,4,4,4,4,4,  
4,4,4

SQL 186,18,18,18,12,12,12,8,8,8,8,8,8,4,4,4,  
4,4,4,4,4,4,  
4,4,4

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

SEQ 1 GXGGGXGGGX GGGXGGGF  
=====

HITS AT: 15-18

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 134:147856

L4 ANSWER 7 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 273944-81-3 REGISTRY  
CN L-Phenylalanine, N-[4-(1,4,7,10-tetraazacyclododec-1-ylmethyl)benzoyl]glycylglycylglycyl-4-isothiocyanato- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)  
SQL 4  
SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 133:28087

L4 ANSWER 8 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 273944-80-2 REGISTRY  
CN L-Phenylalanine, N-[4-(1,4,8,11-tetraazacyclotetradec-1-ylmethyl)benzoyl]glycylglycylglycyl-4-isothiocyanato- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)  
SQL 4  
SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 133:28087

L4 ANSWER 9 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 251459-42-4 REGISTRY  
CN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycylglycylglycyl-N-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location | description                        |
|--------------|----------|------------------------------------|
| modification | Gly-1    | (1,1-dimethylethoxy) carbonyl<Boc> |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:15631

L4 ANSWER 10 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 251459-40-2 REGISTRY  
 CN L-Phenylalaninamide, glycyglycyglycyl-N-[4-[[[[[(1S,9S)-9-ethyl-5-fluoro-2,3,9,10,13,15-hexahydro-9-hydroxy-4-methyl-10,13-dioxo-1H,12H-benzo[de]pyrano[3',4':6,7]indolizino[1,2-b]quinolin-1-yl]amino]carbonyl]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)  
 SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:15631

L4 ANSWER 11 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 251459-38-8 REGISTRY  
 CN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyglycyglycyl-N-[4-[[[[[(1S,9S)-9-ethyl-5-fluoro-2,3,9,10,13,15-hexahydro-9-hydroxy-4-methyl-10,13-dioxo-1H,12H-benzo[de]pyrano[3',4':6,7]indolizino[1,2-b]quinolin-1-yl]amino]carbonyl]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

| type         | location | description                        |
|--------------|----------|------------------------------------|
| modification | Gly-1    | (1,1-dimethylethoxy) carbonyl<Boc> |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:15631

L4 ANSWER 12 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 251459-36-6 REGISTRY  
 CN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyglycyglycyl-N-[4-[[[(4-nitrophenoxy)carbonyl]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

| type         | location | description                        |
|--------------|----------|------------------------------------|
| modification | Gly-1    | (1,1-dimethylethoxy) carbonyl<Boc> |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:15631

L4 ANSWER 13 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 251459-34-4 REGISTRY  
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]glycylglycylglycyl- (9CI)  
(CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location | description                        |
|--------------|----------|------------------------------------|
| modification | Gly-1    | (1,1-dimethylethoxy) carbonyl<Boc> |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:15631

L4 ANSWER 14 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 219721-93-4 REGISTRY  
CN L-Phenylalaninamide, glycylglycylglycyl-4-isothiocyanato- (9CI) (CA INDEX NAME)

NTE modified (modifications unspecified)

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 130:106984

L4 ANSWER 15 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 180737-56-8 REGISTRY  
CN Cyclo(glycylglycylglycyl-4-nitro-L-phenylalanyl) (9CI) (CA INDEX NAME)

NTE cyclic

modified (modifications unspecified)

| type         | location | description |
|--------------|----------|-------------|
| modification | Phe-4    | nitro<N>    |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:156840

REFERENCE 2: 125:204516

L4 ANSWER 16 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 180737-55-7 REGISTRY  
CN L-Phenylalanine, glycylglycylglycyl-4-nitro- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:

CN L-Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-4-nitro-  
NTE modified (modifications unspecified)

| type         | location | description |
|--------------|----------|-------------|
| modification | Phe-4    | nitro<N>    |

SQL 4  
SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:156840

REFERENCE 2: 125:204516

L4 ANSWER 17 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 180737-51-3 REGISTRY  
CN L-Phenylalanine, N-[N-[2-[(aminoacetyl)amino]ethyl]-N-(trifluoroacetyl)glycyl]-4-nitro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | Gly-2    | undetermined modification |
| modification | Gly-3    | trifluoroacetyl<Tfa>      |
| modification | Phe-4    | nitro<N>                  |

SQL 4  
SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 125:204516

L4 ANSWER 18 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 176171-19-0 REGISTRY  
CN L-Phenylalanine, N-[4-(aminosulfonyl)benzoyl]glycylglycylglycyl-4-chloro- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Phenylalanine, N-[N-[N-[N-[4-(aminosulfonyl)benzoyl]glycyl]glycyl]glycyl]-4-chloro-  
NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | Gly-1    | undetermined modification |
| modification | Phe-4    | chloro<Cl>                |

SQL 4  
SQL 4

SEQ 1 GGGF

====



HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 126:141273

REFERENCE 2: 124:317848

L4 ANSWER 19 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 176171-18-9 REGISTRY  
CN L-Phenylalanine, N-[N-[N-[N-[4-(aminosulfonyl)benzoyl]glycyl]glycyl]glycyl  
]-4-fluoro- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location |   | description               |
|--------------|----------|---|---------------------------|
| modification | Gly-1    | - | undetermined modification |
| modification | Phe-4    | - | fluoro<F>                 |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 124:317848

L4 ANSWER 20 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 176171-17-8 REGISTRY  
CN L-Phenylalanine, N-[N-[N-[N-[4-(aminosulfonyl)benzoyl]glycyl]glycyl]glycyl  
]-4-nitro- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location |   | description               |
|--------------|----------|---|---------------------------|
| modification | Gly-1    | - | undetermined modification |
| modification | Phe-4    | - | nitro<N>                  |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 124:317848

L4 ANSWER 21 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 176171-07-6 REGISTRY  
CN L-Phenylalanine, 4-amino-N-[N-[N-[N-[4-(aminosulfonyl)benzoyl]glycyl]glycyl  
]glycyl]- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location |   | description               |
|--------------|----------|---|---------------------------|
| modification | Gly-1    | - | undetermined modification |
| modification | Phe-4    | - | amino<NH2>                |

SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 124:317848

L4 ANSWER 22 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 167861-74-7 REGISTRY  
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]glycylglycylglycyl-4-nitro- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Phenylalanine, N-[N-[N-[N-[(1,1-dimethylethoxy)carbonyl]glycyl]glycyl]glycyl]-4-nitro-  
NTE modified (modifications unspecified)

| type         | location |   | description                        |
|--------------|----------|---|------------------------------------|
| modification | Gly-1    | - | (1,1-dimethylethoxy) carbonyl<Boc> |
| modification | Phe-4    | - | nitro<N>                           |

SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 132:156840

REFERENCE 2: 125:204516

REFERENCE 3: 123:225940

L4 ANSWER 23 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 167861-64-5 REGISTRY  
CN 1,4,7,10-Tetraazacyclododecane-2,5,8,11-tetrone, 3-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)  
NTE cyclic  
modified (modifications unspecified)

| type         | location |   | description |
|--------------|----------|---|-------------|
| modification | Phe-4    | - | nitro<N>    |

SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 123:225940

L4 ANSWER 24 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 167861-63-4 REGISTRY  
 CN 1,4,7,10-Tetraazacyclododecane-2,5,8,11-tetrone, 9-[(4-nitrophenyl)methyl]-  
 1-(trifluoroacetyl)- (9CI) (CA INDEX NAME)  
 NTE cyclic  
 modified (modifications unspecified)

| type         | location |   | description          |
|--------------|----------|---|----------------------|
| modification | Gly-3    | - | trifluoroacetyl<Tfa> |
| modification | Phe-4    | - | nitro<N>             |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 123:225940

L4 ANSWER 25 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 167861-62-3 REGISTRY  
 CN L-Phenylalanine, N-[N-[2-[(aminoacetyl)amino]ethyl]-N-  
 (trifluoroacetyl)glycyl]-4-nitro- (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

| type         | location |   | description               |
|--------------|----------|---|---------------------------|
| modification | Gly-2    | - | undetermined modification |
| modification | Gly-3    | - | trifluoroacetyl<Tfa>      |
| modification | Phe-4    | - | nitro<N>                  |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 125:204516

REFERENCE 2: 123:225940

L4 ANSWER 26 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 167861-61-2 REGISTRY  
 CN L-Phenylalanine, N-[N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]ami  
 no]ethyl]-N-(trifluoroacetyl)glycyl]-4-nitro-, 1,1-dimethylethyl ester  
 (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

| type         | location |   | description                        |
|--------------|----------|---|------------------------------------|
| modification | Gly-1    | - | (1,1-dimethylethoxy) carbonyl<Boc> |
| modification | Gly-2    | - | undetermined modification          |
| modification | Gly-3    | - | trifluoroacetyl<Tfa>               |
| modification | Phe-4    | - | nitro<N>                           |

SQL 4  
 SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 125:204516

REFERENCE 2: 123:225940

L4 ANSWER 27 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 165682-42-8 REGISTRY

CN L-Phenylalanine, N-[N-[N-[N-[4-(aminosulfonyl)benzoyl]glycyl]glycyl]glycyl  
]- (9CI) (CA INDEX NAME)

NTE modified (modifications unspecified)

| type         | ----- | location | ----- | description               |
|--------------|-------|----------|-------|---------------------------|
| modification | Gly-1 | -        |       | undetermined modification |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 124:317848

REFERENCE 2: 123:106470

L4 ANSWER 28 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 149226-84-6 REGISTRY

CN L-Phenylalaninamide, glycylglycylglycyl-4-nitro-, mono(trifluoroacetate)  
(9CI) (CA INDEX NAME)

NTE modified

| type          | ----- | location | ----- | description               |
|---------------|-------|----------|-------|---------------------------|
| terminal mod. | Phe-4 | -        |       | C-terminal amide          |
| modification  | -     | -        |       | undetermined modification |
| modification  | Phe-4 | -        |       | nitro<N>                  |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

RN 149226-84-6 REGISTRY

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

SEQ 1 GGGF

====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 119:90207

L4 ANSWER 29 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 149226-83-5 REGISTRY  
CN L-Phenylalaninamide, glycylglycylglycyl-4-nitro- (9CI) (CA INDEX NAME)  
NTE modified

| type          | location |   | description      |
|---------------|----------|---|------------------|
| terminal mod. | Phe-4    | - | C-terminal amide |
| modification  | Phe-4    | - | nitro<N>         |

SQL 4  
SQL 4

SEQ 1 GGGF

====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

L4 ANSWER 30 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 149206-85-9 REGISTRY  
CN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycylglycylglycyl-4-nitro- (9CI) (CA INDEX NAME)  
NTE modified

| type          | location |   | description                        |
|---------------|----------|---|------------------------------------|
| terminal mod. | Phe-4    | - | C-terminal amide                   |
| modification  | Gly-1    | - | (1,1-dimethylethoxy) carbonyl<Boc> |
| modification  | Phe-4    | - | nitro<N>                           |

SQL 4  
SQL 4

SEQ 1 GGGF

====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 119:90207

L4 ANSWER 31 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 135612-66-7 REGISTRY  
CN L-Phenylalaninamide, N-carboxyglycylglycylglycyl-N-(4-nitrophenyl)- (9CI)  
(CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location |   | description               |
|--------------|----------|---|---------------------------|
| modification | Gly-1    | - | undetermined modification |

SQL 4  
SQL 4

SEQ 1 GGGF

====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 116:17641

L4 ANSWER 32 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 134002-70-3 REGISTRY  
CN L-Phenylalaninamide, glycylglycylglycyl-N-[4-(ethoxycarbonyl)phenyl]-,  
monohydrochloride (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | -        | undetermined modification |

SQL 4  
SQL 4

SEQ 1 GGGF

====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 114:240639

L4 ANSWER 33 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 133954-78-6 REGISTRY  
CN L-Phenylalaninamide, glycylglycylglycyl-N-[4-(ethoxycarbonyl)phenyl]-  
(9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

SQL 4  
SQL 4

SEQ 1 GGGF

====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 114:240639

L4 ANSWER 34 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 110672-90-7 REGISTRY  
CN L-Phenylalanine, N-[N-[N-(9H-pyrido[3,4-b]indol-3-ylcarbonyl)glycyl]glycyl]glycyl]-, methyl ester (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 9H-Pyrido[3,4-b]indole, L-phenylalanine deriv.  
NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | Gly-1    | undetermined modification |

SQL 4  
SQL 4

SEQ 1 GGGF

====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 107:198895

L4 ANSWER 35 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 104724-44-9 REGISTRY  
CN L-Phenylalanine, N-[N-[N-[(5-fluoro-3,4-dihydro-2,4-dioxo-1(2H)-  
pyrimidinyl)acetyl]glycyl]glycyl]- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)  
SQL 4  
SQL 4

SEQ 1 GGGF  
=====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 105:173025

L4 ANSWER 36 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 90409-74-8 REGISTRY  
CN L-Phenylalaninamide, N-(2-methyl-1-oxo-2-propenyl)glycylglycylglycyl-N-(4-  
nitrophenyl)-, polymer with 2-methyl-2-propenoic acid (9CI) (CA INDEX  
NAME)  
OTHER CA INDEX NAMES:  
CN 2-Propenoic acid, 2-methyl-, polymer with N-(2-methyl-1-oxo-2-  
propenyl)glycylglycylglycyl-N-(4-nitrophenyl)-L-phenylalaninamide (9CI)  
NTE homopolymer  
modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | -        | undetermined modification |
| modification | Gly-1    | 2-methyl-1-oxo-2-propenyl |

SQL 4  
SQL 4

SEQ 1 GGGF  
=====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

RN 90409-74-8 REGISTRY

SEQ 1 GGGF  
=====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

SEQ 1 GGGF  
=====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 101:12062

L4 ANSWER 37 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 84814-48-2 REGISTRY  
CN Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-, methyl ester, monoacetate

(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-, methyl ester, monoacetate  
NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | -        | undetermined modification |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

RN 84814-48-2 REGISTRY

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 98:107729

L4 ANSWER 38 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 84814-47-1 REGISTRY

CN Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-, methyl ester (9CI) (CA  
INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-, methyl ester  
NTE modified (modifications unspecified)

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 98:107729

L4 ANSWER 39 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 78682-74-3 REGISTRY

CN L-Phenylalanine, N-[N-[N-(N-acetylglycyl)glycyl]glycyl]-, methyl ester  
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN N-Acetylglycylglycylglycyl-L-phenylalanine methyl ester  
NTE modified

| type          | location | description |
|---------------|----------|-------------|
| terminal mod. | Gly-1    | N-acetyl    |



SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 116:17641

REFERENCE 2: 95:76069

L4 ANSWER 40 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 78682-72-1 REGISTRY  
CN L-Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-, methyl ester,  
monohydrobromide (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | -        | undetermined modification |

SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 95:76069

L4 ANSWER 41 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 75853-32-6 REGISTRY  
CN L-Phenylalanine, glycylglycylglycyl- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Alanine, N-[N-(N-glycylglycyl)glycyl]-3-phenyl- (7CI)  
CN L-Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-  
OTHER NAMES:  
CN 6: PN: WO02087632 PAGE: 21 unclaimed sequence  
CN 88: PN: WO03045309 SEQID: 2 unclaimed sequence  
SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 139:30773

REFERENCE 2: 137:348514

REFERENCE 3: 132:326152

REFERENCE 4: 94:1489

REFERENCE 5: 61:69405

L4 ANSWER 42 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 75501-77-8 REGISTRY  
 CN L-Phenylalaninamide, N-[(phenylmethoxy)carbonyl]glycylglycylglycyl- (9CI)  
 (CA INDEX NAME)  
 OTHER NAMES:  
 CN Z-Gly-Gly-Gly-Phe-NH2  
 NTE modified

| type          | location | description                |
|---------------|----------|----------------------------|
| terminal mod. | Phe-4    | C-terminal amide           |
| modification  | Gly-1    | (phenylmethoxy)carbonyl<Z> |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 93:217111

L4 ANSWER 43 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 74578-54-4 REGISTRY  
 CN L-Phenylalaninamide, N-[(phenylmethoxy)carbonyl]glycylglycylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

| type         | location | description                |
|--------------|----------|----------------------------|
| modification | Gly-1    | (phenylmethoxy)carbonyl<Z> |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 93:95630

L4 ANSWER 44 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 74569-71-4 REGISTRY  
 CN L-Phenylalaninamide, glycylglycylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

SQL 4  
 SQL 4

SEQ 1 GGGF  
 =====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 93:101418

REFERENCE 2: 93:95630

L4 ANSWER 45 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 67877-92-3 REGISTRY  
 CN L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)glycylglycylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

| type         | location | description                |
|--------------|----------|----------------------------|
| modification | Gly-1 -  | 3-carboxy-1-oxopropyl<Suc> |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 93:95630

REFERENCE 2: 89:175672

L4 ANSWER 46 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 61435-98-1 REGISTRY

CN L-Phenylalaninamide, N-(2-methyl-1-oxo-2-propenyl)glycylglycylglycyl-N-(4-nitrophenyl)-, polymer with N-(2-hydroxypropyl)-2-methyl-2-propenamide (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Propenamide, N-(2-hydroxypropyl)-2-methyl-, polymer with N-(2-methyl-1-oxo-2-propenyl)glycylglycylglycyl-N-(4-nitrophenyl)-L-phenylalaninamide (9CI)

NTE homopolymer

modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | -        | undetermined modification |
| modification | Gly-1 -  | 2-methyl-1-oxo-2-propenyl |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

RN 61435-98-1 REGISTRY

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 114:192393

REFERENCE 2: 101:12062

REFERENCE 3: 86:13107

L4 ANSWER 47 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 61435-72-1 REGISTRY  
CN L-Phenylalaninamide, N-(2-methyl-1-oxo-2-propenyl)glycylglycylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | Gly-1    | 2-methyl-1-oxo-2-propenyl |

SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 86:13107

L4 ANSWER 48 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 58688-92-9 REGISTRY  
CN L-Phenylalanine, N-[N-(N-benzoylglycyl)glycyl]glycyl- (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

| type         | location | description |
|--------------|----------|-------------|
| modification | Gly-1    | benzoyl<Bz> |

SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 112:3104

REFERENCE 2: 84:101503

L4 ANSWER 49 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 47458-92-4 REGISTRY  
CN L-Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-, methyl ester (9CI) (CA INDEX NAME)  
NTE modified (modifications unspecified)

SQL 4  
SQL 4

SEQ 1 GGGF  
====  
HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 113:41278

L4 ANSWER 50 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 37923-00-5 REGISTRY  
 CN L-Phenylalanine, N-[N-[N-[N-[5-(dimethylamino)-1-naphthalenyl]sulfonyl]glycyl]glycyl]glycyl]- (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN N-Dansylglycylglycylglycyl-L-phenylalanine  
 NTE modified (modifications unspecified)

| type         | location | description                                |
|--------------|----------|--|
| modification | Gly-1    | [5-(dimethylamino)-1-naphthalenyl]sulfonyl |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 98:139670

REFERENCE 2: 77:98334

L4 ANSWER 51 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 33492-41-0 REGISTRY  
 CN Alanine, N-[N-(N-glycylglycyl)glycyl]-3-phenyl-, methyl ester, monoacetate, L- (8CI) (CA INDEX NAME)  
 NTE modified (modifications unspecified)

| type         | location | description               |
|--------------|----------|---------------------------|
| modification | -        | undetermined modification |

SQL 4  
 SQL 4

SEQ 1 GGGF  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

RN 33492-41-0 REGISTRY

SEQ 1 GGGF  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

SEQ 1 GGGF  
 HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 75:98805

L4 ANSWER 52 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 33374-78-6 REGISTRY

CN L-Phenylalanine, N-[N-[N-[N-[(phenylmethoxy)carbonyl]glycyl]glycyl]glycyl]-  
, methyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Alanine, N-[N-[N-(N-carboxyglycyl)glycyl]glycyl]-3-phenyl-, N-benzyl  
methyl ester (7CI)

CN Alanine, N-[N-[N-(N-carboxyglycyl)glycyl]glycyl]-3-phenyl-, N-benzyl  
methyl ester, L- (8CI)

NTE modified (modifications unspecified)

| type         | location | description                 |
|--------------|----------|-----------------------------|
| modification | Gly-1 -  | (phenylmethoxy) carbonyl<Z> |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 95:76069

REFERENCE 2: 75:98805

REFERENCE 3: 61:69405

L4 ANSWER 53 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 26108-22-5 REGISTRY

CN Alanine, N-[N-[N-(N-carboxyglycyl)glycyl]glycyl]-3-phenyl-, N-benzyl  
3-(4-pyridyl)propyl ester, L- (8CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 4-Pyridinepropanol, ester with N-[N-[N-(N-carboxyglycyl)glycyl]glycyl]-3-  
phenyl-L-alanine N-benzyl ester (8CI)

NTE modified (modifications unspecified)

| type         | location | description                 |
|--------------|----------|-----------------------------|
| modification | Gly-1 -  | (phenylmethoxy) carbonyl<Z> |

SQL 4

SQL 4

SEQ 1 GGGF

====

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 72:18693

L4 ANSWER 54 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 25894-99-9 REGISTRY

CN Phenylalanine, N-[N-(N-glycylglycyl)glycyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Alanine, N-[N-(N-glycylglycyl)glycyl]-3-phenyl-, DL- (8CI)

CN DL-Phenylalanine, N-[N-(N-glycylglycyl)glycyl]-

OTHER NAMES:

CN Triglycyl-DL-phenylalanine

SQL 4

SQL 4

SEQ 1 GGGF

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 73:74039

L4 ANSWER 55 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 24848-63-3 REGISTRY

CN L-Phenylalanine, N-[N-[N-[N-[(phenylmethoxy)carbonyl]glycyl]glycyl]glycyl]-  
(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Alanine, N-[N-[N-(N-carboxyglycyl)glycyl]glycyl]-3-phenyl-, N-benzyl ester  
(7CI)

NTE modified (modifications unspecified)

| type         | location | description                 |
|--------------|----------|-----------------------------|
| modification | Gly-1    | (phenylmethoxy) carbonyl<Z> |

SQL 4

SQL 4

SEQ 1 GGGF

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 117:70314

REFERENCE 2: 104:6163

REFERENCE 3: 84:101503

REFERENCE 4: 61:69405

L4 ANSWER 56 OF 56 REGISTRY COPYRIGHT 2003 ACS on STN

RN 3017-43-4 REGISTRY

CN 1,4,7,10-Tetraazacyclododecane-2,5,8,11-tetrone, 3-benzyl- (7CI, 8CI) (CA  
INDEX NAME)

NTE cyclic

SQL 4

SQL 4

SEQ 1 GGGF

HITS AT: 1-4

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

REFERENCE 1: 62:52017

REFERENCE 2: 62:52016